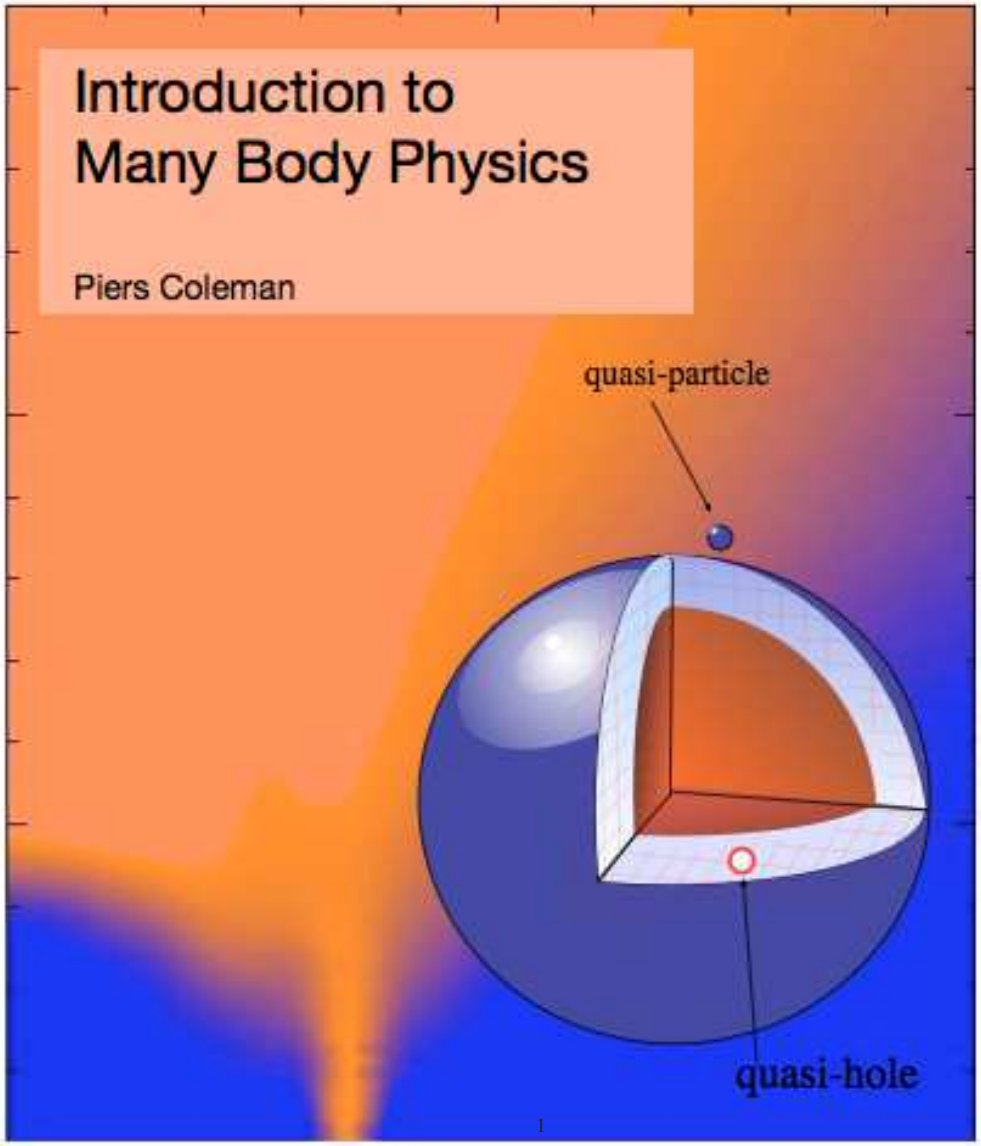
Introduction to
Many Body Physics
Piers Coleman
quasi-particle
quasi-hole

Contents

Chapter 1

Introduction

This monogram is written with the graduate student in mind. I had in mind to write a short, crisp book that would introduce my students to the basic ideas and concepts behind many body physics. At the same time, I felt very strongly that I should like to share my excitement with this field, for without feeling the thrill of entering uncharted territory, I do not think one has the motivation to learn and to make the passage from learning to research.

Traditionally, as physicists we ask "what are the microscopic laws of nature ?", often proceeding with the brash certainty that once revealed, these laws will have such profound beauty and symmetry, that the properties of the universe at large will be self-evident. This basic philosophy can be traced from the earliest atomistic philosophies of Democritus, to the most modern quests to unify quantum mechanics and gravity.

The dreams and aspirations of many body physics interwine the atomistic approach with a complimentary philosophy- that of *emergent phenomena*. From this view, fundamentally new kinds of phenomena emerge within complex assemblies of particles which can not be anticipated from an à priori knowledge of the microscopic laws of nature. Many body physics aspires to synthesize from the microscopic laws, new principles that govern the macroscopic realm, asking

What new principles and laws emerge as we make the journey from the microscopic to the macroscopic?

This is a comparatively new scientific philosophy. Darwin was the perhaps the first to seek an understanding of emergent laws of nature. Following in his footsteps, Boltzmann was probably the first physicist to appreciate the need to understand how emergent principles are linked to microscopic physics, From Boltzmann's biography[1], we learn that he was strongly influenced and inspired by Darwin. In more modern times, a strong advocate of this philosophy has been Philip Anderson, who first introduced the phrase "emergent phenomenon" into physics[2]. In an influential article entitled "More is different" written in 1967,[2] P.W. Anderson captured the philosophy of emergence, writing

"The behavior of large and complex aggregations of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear, and the understanding of the new behaviors requires research which I think is as fundamental in its nature as any other."

P. W. Anderson from "More is Different" , 1967.

In an ideal world, I would hope that from this short course your knowledge of many body techniques will grow hand-in-hand with an appreciation of the motivating philsophy. In many ways, this dual track is essential, for often, one needs both inspiration and overview to steer one lightly through the formalism, without getting bogged down in mathematical quagmires.

I have tried in the course of the book to mention aspects of the history of the field. We often forget that act of discovering the laws of nature is a very human and very passionate one. Indeed, the act of creativity in physics research is very similar to the artistic process. Sometimes, scientific and artistic revolution even go hand in hand - for the desire for change and revolution often crosses between art and sciences[3]. I think it is important for students to gain a feeling of this passion behind the science, and for this reason I have often included a few words about the people and the history behind the ideas that appear in this text. There are unfortunately, very few texts that tell the history of many body physics. Pais' book "Inward Bound" has some important chapters on the early stages of many body physics. A few additional references are included at the end of this chapter[4, 5, 6, 7]

There are several texts that can be used as reference books in parallel with this monogram, of which a few deserve special mention. The student reading this book will need to consult standard references on condensed matter and statistical mechanics. Amongst the various references let me recommend "Statistical Physics Part II" by Landau and Pitaevksii[8]. For a conceptual underpining of the concepts of condensed matter physics, may I refer you to the Anderson's classic "Basic Notions in Condensed Matter Physics"[9]. Amongst the classic references to many body physics let me mention "AGD"[10], Methods of Quantum Field Theory by Abrikosov, Gorkhov and Dzyaloshinksi. This is the text that drove the quantum many body revolution of the sixties and seventies, yet it is still very relevant today, if rather terse. Other many body texts which introduce the reader to the Green function approach to many body physics include "Many Particle Physics" by G. Mahan[11], notable for the large number of problems he provides, "Green Functions for "Green's functions for Solid State Physics" by Doniach and Sondheimer[12] and the very light introduction to the subject "Feynman diagrams in Solid State Physics" by Richard Mattuck[13]. Amongst the more recent treatments, let me note Alexei Tsvelik's "Quantum Field Theory" in Condensed Matter Physics"[14], provides a wonderful introduction to many of the more modern approaches to condensed matter physics, including an introduction to bosonization and conformal field theory. As a reference to the early developments of many body physics, I recommend "The Many Body Problem", by David Pines[15], which contains a compilation of the classic early papers in the field. Lastly, let me recommend the reader to numerous excellent online reference sources, in addition to the online physics archive http://arXiv.org, let me mention writing include online lecture notes on many body theory by Ben Simon and Alexander Atlund[16] and lecture notes on Solid State Physics and Many Body Theory by Chetan Nayak[17].

Here is a brief summary of what we will cover:

1. Scales and complexity, where we discuss the gulf of time (T), length-scale (L), particle number (N) and complexity that separates the microscopic from the macroscopic.

2. Second Quantization. Where make the passage from the wavefunction, to the field operator, and introduce the excitation concept.

3. Introducing the fundamental correlator of quantum fields: the Green's functions. Here we develop the tool of Feynman diagrams for visualizing and calculating many body processes.

4. Finite temperature and imaginary time. By replacing $it \to \tau$, $e^{-iHt} \to e^{-T\tau}$, we will see how to extend quantum field theory to finite temperature, where we will find that there is an intimate link between fluctuations and dissipation.

5. The disordered metal. Second quantized treatment of weakly disordered metals: the Drude metal, and the derivation of "Ohm's law" from first principles.

6. Opening the door to Path Integrals, linking the partition function and S-matrix to an integral over all possible time-evolved paths of the many-body system. $Z = \int_{PATH} e^{-S/\hbar}$.

7. The concept of broken symmetry and generalized rigidity, as illustrated by superconductivity and pairing.

8. A brief introduction to the physics of local moment systems

Finally, a brief note on the conventions used in this book. This book uses standard SI notation, which means abandoning some of the notational elegance of cgs units, but brings the book into line with the international standards. Also, following a convention followed in the early Russian texts on physics and many body physics, and by Mahan's many body physics[11], I use the convention that the charge on the electron is

$$e = -1.602\cdots \times 10^{-19}\text{C}$$

In other words $e = -|e|$ denotes the magnitude *and* the sign of the electron charge. This convention minimizes the number of minus signs required. With this notation, the Hamiltonian of an electron in a magnetic field is given by

$$H = \frac{(\mathbf{p} - e\mathbf{A})^2}{2m} + eV$$

where $\mathbf{A}$ is the vector potential and V the electric potential. The magnitude of the electron charge is denoted by $|e|$ in formulae, such as the electron cyclotron frequency $\omega_c = \frac{|e|B}{m}$.

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Chapter 2

Scales and Complexity

We do infact know the microscopic physics that governs all metals, chemistry, materials and possibly life itself. In principle, all can be determined from the many-particle wavefunction

$$\Psi(\vec{x}_1, \vec{x}_2 \ldots \vec{x}_N, t), \tag{2.1}$$

which in turn, is governed by the Schödinger equation[1, 2], written out for identical particles as

$$\left\{ -\frac{\hbar^2}{2m} \sum_{j=1}^{N} \nabla_j^2 + \sum_{i<j} V(\vec{x}_i - \vec{x}_j) + \sum_j U(\vec{x}_j) \right\} \Psi = i\hbar \frac{\partial \Psi}{\partial t} \tag{2.2}$$

[*Schrödinger, 1926]*

There are of course many details that I have omitted- for instance, if we're dealing with electrons then $V(x)$ is the Coulomb interaction potential,

$$V(\vec{x}) = \frac{e^2}{4\pi\epsilon_o} \frac{1}{|\vec{x}|}, \tag{2.3}$$

and $e = -|e|$ is the charge on the electron. In an electromagnetic field we must "gauge" the derivatives $\nabla \to \nabla - i(e/\hbar)\mathbf{A}$, $U(x) \to U(x) + e\Phi(\vec{x})$, where $\vec{A}$ is the vector potential and $\Phi(\vec{x})$ is the electric potential. Also, to be complete, we must discuss spin, the antisymmetry of Ψ under particle exchange and of course, the elastic displacements of the atoms in the crystal. With these provisos, we have every reason to believe that this is the equation that governs the microsopic behavior of materials.

Unfortunately this knowledge is only the beginning. Why? Because at the most pragmatic level, we are defeated by the sheer complexity of the problem. Even the task of solving the Schrödinger equation for modest multi-electron atoms proves insurmountable without bold approximations. The problem facing the condensed matter physicist, with systems involving 10^{23} atoms, is qualitatively more severe. The amount of storage required for numerical solution of Schrodinger equation grows exponentially with the number of particles, so with a macroscopic number of interacting particles

this becomes far more than a technical problem- it becomes one of principle. Indeed, we believe that the gulf between the microscopic and the macroscopic is something qualitative and fundamental, so much so that new types of property emerge in macroscopic systems that we can not anticipate a priori by using brute-force analyses of the Schrödinger equation.

The "Hitchhiker's guide to the Galaxy" [3] describes a super computer called "Deep Thought" that after millions of years spent calculating 'the answer to the ultimate question of life and the universe', reveals it to be 42. Adams' cruel parody of reductionism holds a certain sway in physics today. Our "forty two", is Schroedinger's many body equation: a set of relations that whose complexity grows so rapidly that we can't trace its full consequences to macroscopic scales. All is fine, provided we wish to understand the workings of isolated atoms or molecules up to sizes of about a nanometer, but between the nanometer and the micron, wonderful things start to occur that severely challenge our understanding. Physicists, have coined the term "emergence" from evolutionary biology to describe these phenomena[4, 5, 6, 7].

The pressure of a gas is an example of emergence: it's a co-operative property of large numbers of particles which can not be anticipated from the behavior of one particle alone. Although Newton's laws of motion account for the pressure in a gas, a hundred and eighty years elapsed before Maxwell developed the statistical description of atoms needed to understand pressure.

Let us dwell a little more on this gulf of complexity that separates the microscopic from the macroscopic. We can try to describe this gulf using four main catagories of scale:

- T. Time 10^{15}.
- L. Length 10^7.
- N. Number of particles. 10^{22}
- C Complexity.

2.1 Time scales

We can make an estimate of the characteristic quantum time scale by using the uncertainty principle $\Delta\tau\Delta E \sim \hbar$, so that

$$\Delta\tau \sim \frac{\hbar}{[1eV]} \sim \frac{\hbar}{10^{-19}J} \sim 10^{-15}s, \tag{2.4}$$

Although we know the physics on this timescale, in our macroscopic world, the the characteristic timescale $\sim 1s$, so that

$$\frac{\Delta\tau_{Macro}}{\Delta\tau_{Quantum}} \sim 10^{15}. \tag{2.5}$$

To link quantum, and macroscopic timescales, we must make a leap comparable with an extrapolation from the the timescale of a heart-beat to the age of the universe. (10 *billion yrs* $\sim 10^{17}$ *s*.)

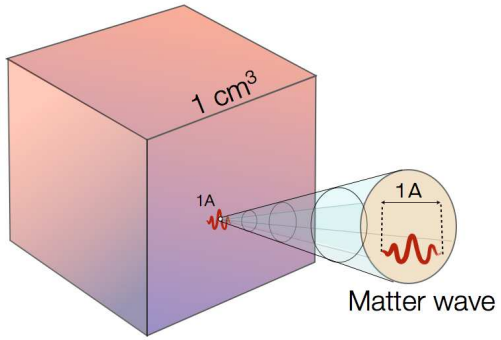

Figure 2.1: The typical size of a de Broglie wave is 10^{-10}m, to be compared with a typical scale 1cm of a macroscopic crystal.

2.2 L: Length scales

An approximate measure for the characteristic length scale in the quantum world is the de Broglie wavelength of an electron in a hydrogen atom,

$$L_{Quantum} \sim 10^{-10} m, \tag{2.6}$$

so

$$\frac{L_{Macroscopic}}{L_{Quantum}} \sim 10^{8} \tag{2.7}$$

At the beginning of the 20th century, the leading philosopher physicist Mach argued to Boltzmann that the atomic hypothesis was metaphysical as one could never envisage a machine with the resolution to image anything so small. Today, this incredible gulf of scale can today be spanned by scanning tunneling microscopes, able to resolve electronic details on the surface of materials with sub-Angstrom resolution.

2.3 N: particle number

To visualize the number of particles in a single mole of substance, it is worth reflecting that a crystal containing a mole of atoms occupies a cube of roughly $1cm^3$. From the quantum perspective, this is

a cube with approximately 100million atoms along each edge. Avagadros number

$$N_{Macroscopic} = 6 \times 10^{23} \sim (100 \text{ million})^3 \tag{2.8}$$

a number which is placed in perspective by reflecting that the number of atoms in a grain of sand is roughly comparable with the number of sand-grains in a 1 mile beach. Notice however that we are used to dealing with inert beaches, where there is no interference between the constituent particles.

2.4 C: Complexity and Emergence.

Real materials are like macroscopic atoms, where the quantum interference amongst the constituent particles gives rise to a range of complexity and diversity that constitutes the largest gulf of all. We can attempt to quantify the "complexity" axis by considering the number of atoms per unit cell of a crystal. Whereas there are roughly 100 stable elements, there are roughly 100^2 stable binary compounds. The number of stable tertiary compounds is conservatively estimated at more than 10^6, of which still only a tiny fraction have been explored experimentally. At each step, the range of diversity increases, and there is reason to believe that at each level of complexity, new types of phenomenon begin to emerge.

But it is really the confluence of length and time scale, particle number and complexity that provides the canvas on which emergent properties develop. While classical matter develops new forms of behavior on large scales, the potential for quantum matter to develop emergent properties is far more startling. For instance, similar atoms of niobium and gold, when scaled up to the micron-scale, form crystals with dramatically different properties. Electrons roam free across gold crystals, forming the conducting fluid that gives it lustrous metallic properties. Up to about 30 nanometers, there is little to distinguish copper and niobium, but beyond this scale, the electrons in niobium pair up into "Cooper pairs" . By the time we reach the scale of a micron, these pairs congregate by the billions into a pair condensate transforming the crystal into an entirely new metallic state: a superconductor, which conducts without resistance, excludes magnetic fields and has the ability to levitate magnets.

Niobium is elemental superconductor, with a transition temperature T_c =9.2K that is pretty typical of conventional "low temperature" superconductors. When experimentalists began to explore the properties of quaternary compounds in the 1980s, they came across the completely unexpected phenomenon of high temperature superconductivity. Even today, two decades later, research has only begun to explore the vast universe of quaternary compounds, and the pace of discovery has not slackened. In the two years preceeding publication of this book, physicists have discovered a new family of iron-based high temperature superconductors, and I'd like to think that before this book goes out of print, many more families will have come to light.

Superconductivity is only a beginning. It is first of all, only one of a large number of broken symmetry states that can develop in "hard" quantum matter. But in assemblies of softer, organic molecules, a tenth of a micron is already enough for the emergence of life. Self-sustaining microbes little more than 200 nanometers in size have been recently been discovered. While we more-or-less understand the principles that govern the superconductor, we do not yet understand those that govern the emergence of life on roughly the same spatial scale[8].

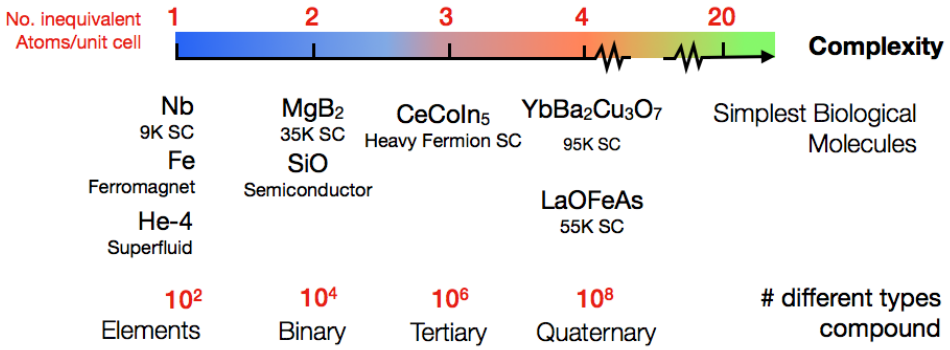

Figure 2.2: Condensed matter of increasing complexity. As the number of inequivalent atoms per "unit cell" grows, the complexity of the material and the potential for new types of behavior grows.

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Chapter 3

Quantum Fields

3.1 Overview

At the heart of quantum many body theory lies the concept of the quantum field. Like a classical field $\phi(x)$, a quantum field is a continuous function of position, excepting now, this variable is an operator $\hat{\phi}(x)$. Like all other quantum variables, the quantum field is in general a strongly fluctuating degree of freedom that only becomes sharp in certain special eigenstates; its function is to add or subtract particles to the system. The appearance of particles or "quanta" of energy $E = \hbar\omega$ is perhaps the greatest single distinction between quantum, and classical fields.

This astonishing feature of quantum fields was first recognized by Einstein, who in 1905 and 1907 made the proposal that the fundamental excitations of continuous media - the electromagnetic field and crystalline matter in particular, are carried by quanta[1, 2, 3, 4], with energy

$$E = \hbar\omega.$$

Einstein made this bold leap in two stages - first by showing that Planck's theory of black-body radiation could be re-interpreted in terms of photons[1, 2], and one year later generalizing the idea to the vibrations inside matter[3] which, he reasoned must also be made up of tiny wave packets of sound that we now call "phonons". From his phonon hypothesis Einstein was able to explain the strong temperature dependence of the specific heat in Diamond - a complete mystery from a classical standpoint. Yet despite these early successes, it took a further two decades before the machinery of quantum mechanics gave Einstein's ideas a concrete mathematical formulation.

Quantum fields are intimately related to the idea of second quantization. First quantization permits us to make the jump from the classical world, to the simplest quantum systems. The classical momentum and position variables are replaced by operators, such as

$$\begin{aligned} E &\rightarrow i\hbar\partial_t, \\ p &\rightarrow \hat{p} = -i\hbar\partial_x, \end{aligned} \tag{3.1}$$

whilst the Poisson bracket which relates canonical conjugate variables is now replaced by the quantum commutator[5, 6]:

$$[x, p] = i\hbar. \tag{3.2}$$

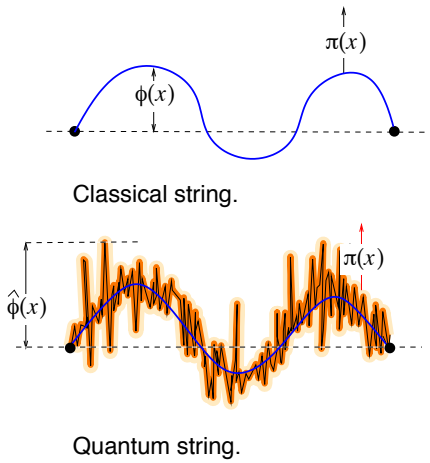

Figure 3.1: Contrasting a classical, and a quantum string.

The commutator is the key to first quantization, and it is the non-commuting property that leads to quantum fluctuations and the Heisenberg uncertainty principle. (See examples). Second quantization permits us to take the next step, extending quantum mechanics to

- Macroscopic numbers of particles.
- Develop an "excitation" or "quasiparticle" description of the low energy physics.
- Describe the dynamical response and internal correlations of large systems.
- To describe collective behavior and broken symmetry phase transitions.

In its simplest form, second quantization elevates classical fields to the status of operators. The simplest example is the quantization of a classical string, as shown in Fig. 3.1. Classically, the string is described by a smooth field $\phi(x)$ which measures the displacement from equilibrium, plus the conjugate field $\pi(x)$ which measures the transverse momentum per unit length. The classical Hamiltonian is

$$H = \int dx \left[\frac{T}{2} (\nabla_x \phi(x))^2 + \frac{1}{2\rho} \pi(x)^2 \right] \tag{3.3}$$

where T is the tension in the string and ρ the mass per unit length. In this case, second-quantization is accomplished by imposing the canonical commutation relations

$$[\phi(x), \pi(y)] = i\hbar\delta(x - y), \qquad \textbf{Canonical commutation relation} \tag{3.4}$$

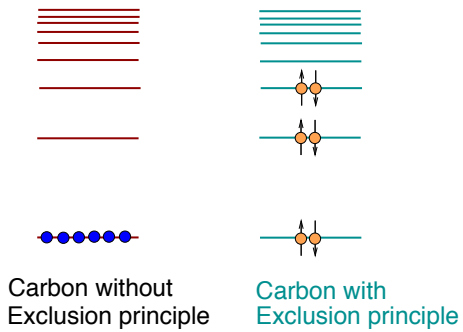

Figure 3.2: Without the exclusion principle, all electrons would occupy the same atomic orbital. There would be no chemistry, no life.

In this respect, second-quantization is no different to conventional quantization, except that the degrees of freedom are defined continuously throughout space. The basic method I have just described works for describing collective fields, such as sound vibrations, or the electromagnetic field, but we also need to know how to develop the field theory of identical particles, such as an electron gas in a metal, or a fluid of identical Helium atoms.

For particle fields, the process of second-quantization is more subtle, for here we the underlying fields have no strict classical counterpart. Historically, the first steps to dealing with such many particle systems were made in atomic physics. In 1925 Pauli proposed his famous "exclusion principle"[7] to account for the diversity of chemistry, and the observation that atomic spectra could be understood only if one assumed there was no more than one electron per quantum state. (Fig. 3.2.) A year later, Dirac and Fermi examined the consequences of this principle for a gas of particles, which today we refer to as "fermions". Dirac realized that the two fundamental varieties of particle- fermions and bosons could be related to the parity of the many-particle wavefunction under particle exchange[8]

$$\Psi(\text{particle at A, particle at B}) = e^{i\Theta}\Psi(\text{particle at B, particle at A}) \tag{3.5}$$

If one exchanges the particles twice, the total phase is $e^{2i\Theta}$. If we are to avoid a many-valued wavefunction, then we must have

$$e^{2i\Theta} = 1 \Rightarrow e^{i\Theta} = \pm 1 \begin{cases} \text{bosons} \\ \text{fermions} \end{cases} \tag{3.6}$$

The choice of $e^{i\Theta} = 1$ leads to a wavefunction which is completely antisymmetric under particle

exchange, which immediately prevents more than one particle in a given quantum state. [1]

In 1927, Jordan and Klein realized that to cast physics of a many body system into a more compact form, one needs to introduce an operator for the particle itself-the field operator. With their innovation, it proves possible to unshackle ourselves from the many body wavefunction. The particle field

$$\hat{\psi}(x) \tag{3.7}$$

operator can be very loosely regarded as a quantization of the one-body Schrodinger wavefunction. Jordan and Klein[9] proposed that the particle field, and its complex conjugate are conjugate variables. With this insight, the second-quantization of bosons is achieved by introducing a non-zero commutator between the particle field, and its complex conjugate. The new quantum fields that emerge play the role of creating, and destroying particles (see below)

$$\underbrace{\psi(x), \psi^*(x)}_{\text{1 ptcle wavefunction}} \xrightarrow{[\psi(x), \psi^\dagger(y)] = \delta(x-y)} \underbrace{\hat{\psi}(x), \hat{\psi}^\dagger(x)}_{\text{destruction /creation operator}} \text{ Bosons} \tag{3.8}$$

For fermions, the existence of an antisymmetric wavefunction, means that particle fields must *anti-commute*, i.e

$$\psi(x)\psi(y) = -\psi(y)\psi(x), \tag{3.9}$$

a point first noted by Jordan, and then developed by Jordan and Wigner[**?**]. The simplest example of anticommuting operators, is provided by the Pauli matrices: we are now going to have to get used to a whole continuum of such operators! Jordan and Wigner realized that the second-quantization of fermions requires that the the non-trivial commutator between conjugate particle fields must be replaced by an anticommutator

$$\underbrace{\psi(x), \psi^*(x)}_{\text{1 ptcle wavefunction}} \xrightarrow{\{\psi(x), \psi^\dagger(y)\} = \delta(x-y)} \underbrace{\hat{\psi}(x), \hat{\psi}^\dagger(x)}_{\text{destruction /creation operator}} \text{ Fermions.} \tag{3.10}$$

The operation $\{a,\ b\} = ab + ba$ denotes the anticommutator. Remarkably, just as bosonic physics derives from commutators, fermionic physics derives from an algebra of anticommutators.

How real is a quantum field and what is its physical significance? To begin to to get a feeling of its meaning, let us look at some key properties. The transformation from wavefunction, to operator also extends to more directly observable quantities. Consider for example, the electron probability density $\rho(x) = \psi^*(x)\psi(x)$ of a one-particle wavefunction $\psi(x)$. By elevating the wavefunction to the status of a field operator, we obtain

$$\rho(x) = |\psi(x)|^2 \rightarrow \hat{\rho}(x) = \hat{\psi}^\dagger(x)\hat{\psi}(x), \tag{3.11}$$

which is the density *operator* for a many body system. Loosely speaking, the squared magnitude of the quantum field represents the density of particles

[1] In dimensions below three, it is possible to have wavefunctions with several Reimann sheets, which gives rise to the concept of fractional statistics and "anyons".

Another aspect of the quantum field we have to understand, is its relationship to the many-body wavefunction. This link depends on a new concept, the "vacuum". This unique state, denoted by $|0\rangle$ is devoid of particles, and for this reason it is the only state for which there is no amplitude to destroy a particle so

$$\psi(x)|0\rangle = 0. \qquad \text{The vacuum} \tag{3.12}$$

We shall see that as a consequence of the canonical algebra, the creation operator $\hat{\psi}^\dagger(x)$ increments the number of particles by one, *creating* a particle at x, so that

$$|x_1\rangle = \psi^\dagger(x_1)|0\rangle \tag{3.13}$$

is a single particle at x_1,

$$|x_1, \ldots x_N\rangle = \psi^\dagger(x_N)\ldots\psi^\dagger(x_1)|0\rangle \tag{3.14}$$

is the N-particle state with particles located at $x_1 \ldots x_N$ and

$$\langle x_1, \ldots x_N| = \langle 0|[\psi^\dagger(x_N)\ldots\psi^\dagger(x_1)]^\dagger = \langle 0|\psi(x_1)\ldots\psi(x_N) \tag{3.15}$$

is its conjugate "bra" vector. The wavefunction of an N particle state, $|N\rangle$ is given by the overlap of $\langle x_1, \ldots x_N|$ with $|N\rangle$:

$$\psi(x_1, \ldots x_N) = \langle x_1, \ldots x_N|N\rangle = \langle 0|\psi(x_1)\ldots\psi(x_N)|N\rangle \tag{3.16}$$

So many body wavefunctions correspond to matrix elements of the quantum fields. From this link we can see that the exchange symmetry under particle exchange is directly linked to the exchange algebra of the field operators. For Bosons and Fermions respectively, we have

$$\langle 0|\ldots\psi(x_r)\psi(x_{r+1})\ldots|N\rangle = \pm\langle 0|\ldots\psi(x_{r+1})\psi(x_r)\ldots|N\rangle \tag{3.17}$$

(where + refers to Bosons, −to fermions), so that

$$\psi(x_r)\psi(x_{r+1}) = \pm\psi(x_{r+1})\psi(x_r) \tag{3.18}$$

From this we see that Bosonic operators commute, but fermionic operators must *anticommute*. Thus it is the exchange symmetry of identical quantum particles that dictates the commuting, or anticommuting algebra of the associated quantum fields.

Unlike a classical field, quantum fields are in a state of constant fluctuation. This applies to both collective fields, as in the example of the string in Fig. 3.1, and to quantum fluids. Just as the commutator between position and momentum gives rise to the uncertainty principle: $[x, p] = i\hbar \longrightarrow \Delta x\Delta p \gtrsim \hbar$, the canonical commutation, or anticommutation relations give rise to a similar relation between the amplitude and phase of the quantum field. Under certain conditions the fluctuations of a quantum field can be eliminated, and in these extreme limits, the quantum field begins to take on a tangible classical existence. In a bose superfluid for example, the quantum field becomes a sharp variable, and we can really ascribe a meaning to the expectation of the quantum field

$$\langle\psi(x)\rangle = \sqrt{\rho_s}e^{i\theta} \tag{3.19}$$

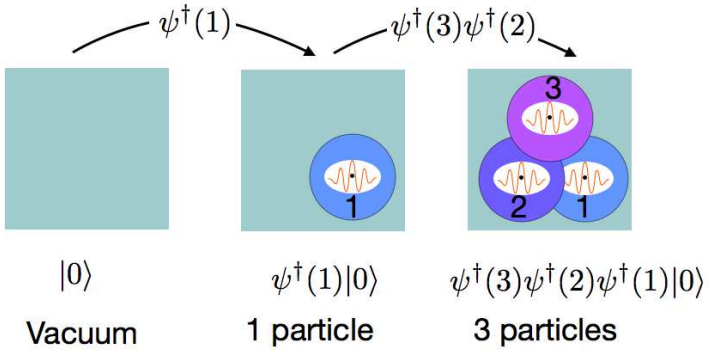

Figure 3.3: Action of creation operator on vacuum to create (i) a one particle and (ii) a three particle state

where ρ_s measures the density of particles in the superfluid condensate. We shall see that there is a completely parallel uncertainty relation between the phase and density of quantum fields,

$$\Delta N\Delta\theta \gtrsim 1 \tag{3.20}$$

where θ is the average phase of a condensate and N the number of particles it contains. When N is truly macroscopic, the uncertainty in the phase may be made arbitrarily small, so that in a Bose superfluid, the phase becomes sufficiently well defined that it becomes possible to observe interference phenomenon! Similar situations arise inside a Laser, where the phase of the electromagnetic field becomes well-defined, or a superconductor, where the phase of the electrons in the condensate becomes well defined.

In the next two chapters we shall go back and see how all these features appear systematically in the context of "free field theory". We shall begin with collective bosonic fields, which behave as a dense ensemble of coupled Harmonic oscillators. In the next chapter, we shall move to conserved particles, and see how the exchange symmetry of the wavefunction leads to the commutation, and anticommutation algebra of bose and Fermi fields. We shall see how this information enables us to completely solve the properties of a non-interacting Bose, or Fermi fluid.

It is the non-commuting properties of quantum fields that generate their intrinsic "*graininess*". Because of this, quantum fields, though nominally continuous degrees of freedom, can always be

decomposed in terms of a discrete particular content. The action of a collective field involves the creation of a wavepacket centered at x by both the creation, and destruction of quanta, schematically,

$$\phi(x) = \sum_{\mathbf{k}} \left[\begin{array}{c} \text{boson creation,} \\ \text{momentum -k} \end{array} + \begin{array}{c} \text{boson destruction} \\ \text{momentum k} \end{array} \right] e^{-i\mathbf{k}\cdot\mathbf{x}}, \tag{3.21}$$

Examples of such quanta, include quanta of sound, or phonons, and quanta of radiation, or photons. In a similar way, the action of a particle creation operator creates a wavepacket of particles at x, schematically,

$$\psi^\dagger(x) = \sum_{\mathbf{k}} \left[\begin{array}{c} \text{particle creation} \\ \text{momentum k} \end{array} \right] e^{-i\mathbf{k}\cdot\mathbf{x}}. \tag{3.22}$$

When the underlying particles develop coherence, the quantum field begins to behave classically. It is the ability of quantum fields to describe continuous classical behavior *and* discrete particulate behavior in a unified way that makes them so very special.

Example. By considering the positivity of the quantity $\langle A(\lambda)^\dagger A(\lambda)\rangle$, where $\hat{A} = \hat{x} + i\lambda p$ and λ is a real number, prove the Heisenberg uncertainty relation $\Delta x \Delta p \geq \frac{\hbar}{2}$.

Example. How does the uncertainty principle prevent the collapse of the Hydrogen atom. Is the uncertainty principle enough to explain the stability of matter?

3.2 Collective Quantum Fields

Here, we will begin to familiarize ourselves with quantum fields by developing the field theory of a free, bosonic field. It is important to realize that a bosonic quantum field is fundamentally nothing more than a set of linearly coupled oscillators, and in particular, so long as the system is linear, the modes of oscillation can always be decomposed into a linear sum of independent normal modes. Each normal mode is nothing more than a simple harmonic oscillator, which provides the basic building block for bosonic field theories.

Our basic strategy for quantizing collective, bosonic fields, thus consists of two basic parts. First, we must reduce the Hamiltonian to its normal modes. For translationally invariant systems, this is just a matter of Fourier transforming the field, and its conjugate momenta. Second, we then quantize the normal mode Hamiltonian as a sum of independent Harmonic oscillators.

$$H(\phi,\pi) \xrightarrow{[F.T.]} \text{Normal Co-ords} \xrightarrow{\phi_q \sim (a_q + a^\dagger_{-q})} H = \sum_q \hbar\omega_q (n_q + \tfrac{1}{2}) \tag{3.23}$$

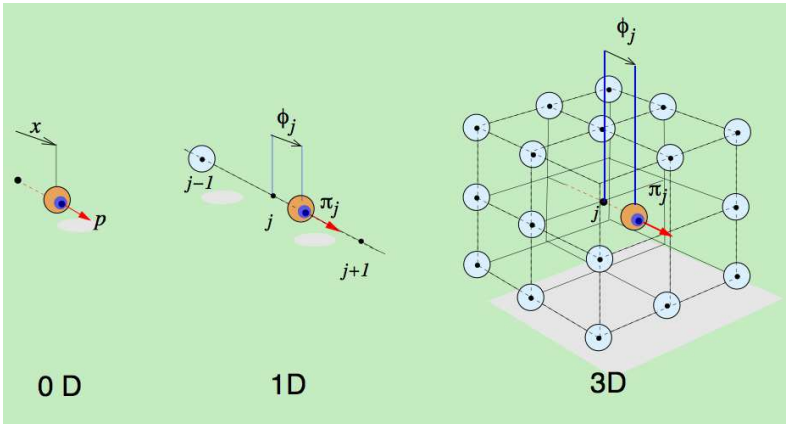

Figure 3.4: Family of zero, one and three-dimensional Harmonic crystals.

The first part of this procedure is essentially identical for both quantum, and classical oscillators. The second-stage is nothing more than the quantization of a single Harmonic oscillator. Consider the family of lattices shown in Figure 3.4. We shall start with a single oscillator at one site. We shall then graduate to one and higher dimensional chain of oscillators, as shown in Fig 3.4.

3.3 Harmonic oscillator: a zero-dimensional field theory

Although the Schrodinger approach is most widely used in first quantization, it is the Heisenberg approach that opens the door to second-quantization. In the Schrödinger approach, one solves the wave-equation

$$\left(\frac{-\hbar^2\partial_x^2}{2m} + \frac{1}{2}m\omega^2 x^2\right)\psi_n = E_n\psi_n \tag{3.24}$$

from which one finds the energy levels are evenly spaced, according to

$$E_n = (n + \frac{1}{2})\hbar\omega, \tag{3.25}$$

where ω is the frequency of the oscillator.

The door to second-quantization is opened by re-interpreting these evenly spaced energy levels in terms of "quanta", each of energy $\hbar\omega$. The nth excited state corresponds to the addition of n

quanta to the ground-state. We shall now see how we can put mathematical meat on these words by introducing an operator "$a^\dagger$" that creates these quanta, so that the n-th excited state is obtained by acting n times on the ground-state with the creation operator.

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle. \tag{3.26}$$

Let us now see how this works. The Hamiltonian for this problem involves conjugate position and momentum operators as follows

$$\left.\begin{array}{rcl} H &=& \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \\ [x,p] &=& i\hbar, \end{array}\right\}. \tag{3.27}$$

In the ground-state, the particle in the Harmonic potential undergoes zero-point motion, with an uncertainty in position and momentum Δp and Δx which satisfy $\Delta x \Delta p \sim \hbar$. Since the zero-point kinetic and potential energies are equal, $\Delta p^2/2m = m\omega^2\Delta x^2/2$, so

$$\Delta x = \sqrt{\frac{\hbar}{m\omega}},\ \Delta p = \sqrt{m\omega\hbar} \tag{3.28}$$

define the scale of zero-point motion. It is useful to define dimensionless position and momentum variables by factoring out the scale of zero-point motion

$$\xi = \frac{x}{\Delta x}, \qquad p_\xi = \frac{p}{\Delta p}. \tag{3.29}$$

One quickly verifies that $[\xi, p_\xi] = i$ are still canonically conjugate, and that now

$$H = \frac{\hbar\omega}{2}\Big[\xi^2 + p_\xi^2\Big]. \tag{3.30}$$

Next, introduce the "creation" and "annihilation" operators

$$\begin{array}{rcll} a^\dagger &=& \frac{1}{\sqrt{2}}(\xi - ip_\xi), & \text{"creation operator"} \\ a &=& \frac{1}{\sqrt{2}}(\xi + ip_\xi), & \text{"annihilation operator".} \end{array} \tag{3.31}$$

Since $[a, a^\dagger] = \frac{-i}{2}([\xi, p_\xi] - [p_\xi, \xi]) = 1$, these operators satisfy the algebra

$$\left.\begin{array}{rcl} [a,a] = [a^\dagger, a^\dagger] &=& 0 \\ [a, a^\dagger] &=& 1. \end{array}\right\} \text{canonical commutation rules} \tag{3.32}$$

It is this algebra which lies at the heart of bosonic physics, enabling us to interpret the creation and annihilation operators as the objects which add, and remove quanta of vibration to and from the system.

To follow the trail further, we rewrite the Hamiltonian in terms of a and $a^\dagger$. Since $\xi = (a + a^\dagger)/\sqrt{2}$, $p_\xi = (a - a^\dagger)/\sqrt{2}i$, the core of the Hamiltonian can be rewritten as

$$\xi^2 + p_\xi^2 = a^\dagger a + aa^\dagger \tag{3.33}$$

But $aa^\dagger = a^\dagger a + 1$, from the commutation rules, so that

$$H = \hbar\omega[a^\dagger a + \frac{1}{2}]. \tag{3.34}$$

This has a beautifully simple interpretation. The second term is just the zero-point energy $E_0 = \hbar\omega/2$ The first term contains the "number operator"

$$\hat{n} = a^\dagger a, \qquad \text{"number operator"} \tag{3.35}$$

which counts the number of vibrational quanta added to the ground state. Each of these quanta carries energy $\hbar\omega$.

To see this, we need to introduce the concept of the vacuum, defined as the unique state such that

$$a|0\rangle = 0. \tag{3.36}$$

From (12.133), this state is clearly an eigenstate of H, with energy $E = \hbar\omega/2$. We now assert that the state

$$|N\rangle = \frac{1}{\lambda_N}(a^\dagger)^N|0\rangle \tag{3.37}$$

where λ_N is a normalization constant, contains N quanta.

To verify that $\hat{n}$ counts the number of bosons, we use the commutation algebra to show that $[\hat{n}, a^\dagger] = a^\dagger$ and $[\hat{n}, a] = -a$, or

$$\begin{array}{rcl} \hat{n}a^\dagger &=& a^\dagger(\hat{n}+1) \\ \hat{n}a &=& a(\hat{n}-1) \end{array} \tag{3.38}$$

which means that when $a^\dagger$ or a act on a state, they respectively add, or remove one quantum of energy. Suppose that

$$\hat{n}|N\rangle = N|N\rangle \tag{3.39}$$

for some N, then from (3.38),

$$\hat{n}\, a^\dagger|N\rangle \;=\; a^\dagger(\hat{n}+1)|N\rangle = (N+1)\, a^\dagger|N\rangle \tag{3.40}$$

so that $a^\dagger|N\rangle \equiv |N+1\rangle$ contains $N+1$ quanta. Since (3.39) holds for $N = 0$, it holds for all N. To complete the discussion, let us fix λ_N by noting that from the definition of $|N\rangle$,

$$\langle N-1|aa^\dagger|N-1\rangle = \left(\frac{\lambda_N}{\lambda_{N-1}}\right)^2\langle N|N\rangle = \left(\frac{\lambda_N}{\lambda_{N-1}}\right)^2, \tag{3.41}$$

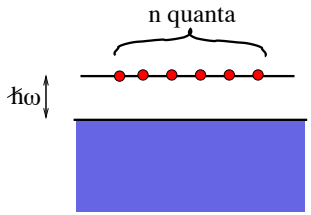

Figure 3.5: Illustrating the excitation picture for a single harmonic oscillator.

but since $aa^\dagger = \hat{n} + 1$, $\langle N-1|aa^\dagger|N-1\rangle = N\langle N-1|N-1\rangle = N$. Comparing these two expressions, it follows that $\lambda_N/\lambda_{N-1} = \sqrt{N}$, and since $\lambda_0 = 1$, $\lambda_N = \sqrt{N!}$.

Summarizing the discussion

$$\begin{aligned} H &= \hbar\omega(\hat{n} + \tfrac{1}{2}) \\ \hat{n} &= a^\dagger a, \qquad \text{“number operator”} \\ |N\rangle &= \tfrac{1}{\sqrt{N!}}(a^\dagger)^N|0\rangle \qquad \text{N-Boson state} \end{aligned} \tag{3.42}$$

Using these results, we can quickly learn many things about the quantum fields a and $a^\dagger$. Let us look at a few examples. First, we can transform all time dependence from the states to the operators by moving to a Heisenberg representation, writing

$$a(t) = e^{iHt/\hbar}ae^{-iHt/\hbar} \qquad \textbf{Heisenberg representation} \tag{3.43}$$

This transformation preserves the canonical commutation algebra, and the form of H. The equation of motion of $a(t)$ is given by

$$\frac{da}{dt} = \frac{i}{\hbar}[H, a(t)] = -i\omega a(t) \tag{3.44}$$

so that the Heisenberg operators are given by

$$\begin{aligned} a(t) &= e^{-i\omega t}a, \\ a^\dagger(t) &= e^{i\omega t}a^\dagger \end{aligned} \tag{3.45}$$

Using these results, we can decompose the original momentum and displacement operators as follows

$$\hat{x}(t) = \Delta x\xi(t) = \frac{\Delta x}{\sqrt{2}}(a(t) + a^\dagger(t)) = \sqrt{\frac{\hbar}{2m\omega}}(ae^{-i\omega t} + a^\dagger e^{i\omega t})$$

$$\hat{p}(t) = \Delta p p_\xi(t) = -i\sqrt{\frac{m\hbar\omega}{2}}(ae^{-i\omega t} - a^\dagger e^{i\omega t}) \tag{3.46}$$

Notice how the displacement operator- a priori a continuous variable, has the action of creating and destroying discrete quanta.

We can use this result to compute the correlation functions of the displacement.

Example 1. *Calculate the autocorrelation function $S(t-t') = \frac{1}{2}\langle 0|\{x(t), x(t')\}|0\rangle$ and the “response” function $R(t-t') = (i/\hbar)\langle 0|[x(t), x(t')]|0\rangle$ in the ground-state of the quantum Harmonic oscillator.*

Solution We may expand the correlation function and response function as follows

$$\begin{aligned} S(t_1 - t_2) &= \frac{1}{2}\langle 0|x(t_1)x(t_2) + x(t_2)x(t_1)|0\rangle \\ R(t_1 - t_2) &= (i/\hbar)\langle 0|x(t_1)x(t_2) - x(t_2)x(t_1)|0\rangle \end{aligned} \tag{3.47}$$

But we may expand $x(t)$ as given in (3.46). The only term which survives in the ground-state, is the term proportional to $aa^\dagger$, so that

$$\langle 0|x(t)x(t')|0\rangle = \frac{\hbar}{2m\omega}\langle 0|aa^\dagger|0\rangle e^{-i\omega(t_1-t_2)} \tag{3.48}$$

Now using (3.47) we obtain

$$\begin{aligned} \frac{1}{2}\langle 0|\{x(t), x(t')\}|0\rangle &= \frac{\hbar}{2m\omega}\cos[\omega(t-t')] \qquad \text{“Correlation function”} \\ -i\langle 0|[x(t), x(t')]|0\rangle &= \frac{1}{m\omega}\sin[\omega(t-t')] \qquad \text{”Response function”} \end{aligned}$$

- We shall later see that $R(t-t')$ gives the response of the ground-state to an applied force $F(t')$, so that at a time t, the displacement is given by

$$\langle x(t)\rangle = \int_{-\infty}^{t} R(t-t')F(t')dt' \tag{3.49}$$

Remarkably, the response function is identical with a classical Harmonic oscillator.

Example 2. *Calculate the number of quanta present in a Harmonic oscillator with characteristic frequency ω, at temperature T.*

To calculate the expectation value of any operator at temperature T, we need to consider an ensemble of systems in different quantum states $|\Psi\rangle = \sum_n c_n|n\rangle$. The expectation value of operator $\hat{A}$ in state $|\Psi\rangle$ is then

$$\langle\hat{A}\rangle = \langle\Psi|\Psi\rangle = \sum_{m,n} c_m^* c_n\langle m|\hat{A}|n\rangle \tag{3.50}$$

In a position basis, this would be

$$\langle \hat{A} \rangle = \sum_{m,n} c_m^* c_n \int dx \psi_m^*(x) A(x) \psi_m(x) \tag{3.51}$$

But now we have to average over the typical state $|\Psi\rangle$ in the ensemble, which gives

$$\overline{\langle \hat{A} \rangle} = \sum_{m,n} \overline{c_m^* c_n} \langle m|\hat{A}|n\rangle = \sum_{m,n} \rho_{mn} \langle m|\hat{A}|n\rangle \tag{3.52}$$

where $\rho_{mn} = \overline{c_m^* c_n}$ is the "density matrix". If the ensemble is in equilibrium with an incoherent heat bath, at temperature T, quantum statistical mechanics asserts that there are no residual phase correlations between the different energy levels, which acquires a Boltzmann distribution

$$\rho_{mn} = \overline{c_m^* c_n} = p_n \delta_{n,m} \tag{3.53}$$

where $p_n = e^{-\beta E_n}/Z$ is the Boltzman distribution, with $\beta = 1/k_B T$, and k_B is Boltzmann's constant. Let us now apply this to our problem, where

$$\hat{A} = \hat{n} = a^\dagger a \tag{3.54}$$

is the number operator. In this case,

$$\langle \hat{n} \rangle = \sum_n (e^{-\beta E_n}/Z) \langle n|\hat{n}|n\rangle = \frac{1}{Z} \sum_n n e^{-\beta E_n} \tag{3.55}$$

To normalize the distribution, we must have $\sum_n p_n = 1$, so that

$$Z = \sum_n e^{-\beta E_n} \tag{3.56}$$

Finally, since $E_n = \hbar\omega(n + \frac{1}{2})$,

$$\langle \hat{n} \rangle = \frac{\sum_n e^{-\beta\hbar\omega(n+\frac{1}{2})} n}{\sum_n e^{-\beta\hbar\omega(n+\frac{1}{2})}} = \frac{\sum_n e^{-\lambda n} n}{\sum_n e^{-\lambda n}}, \qquad \lambda = \beta\hbar\omega. \tag{3.57}$$

The sum in the denominator is a geometric series

$$\sum_n e^{-\lambda n} = \frac{1}{1 - e^{-\lambda}}, \tag{3.58}$$

and the numerator is given by

$$\sum_n e^{-\lambda n} n = -\frac{\partial}{\partial \lambda} \sum_n e^{-\lambda n} = \frac{e^{-\lambda}}{(1 - e^{-\lambda})^2} \tag{3.59}$$

so that

$$\langle \hat{n} \rangle = \frac{1}{e^{\lambda} - 1} = \frac{1}{e^{\beta\hbar\omega} - 1} \tag{3.60}$$

which is the famous Bose-Einstein distribution function.

3.4 Collective modes: phonons

We now extend the discussion of the last section from zero to higher dimensions. Let us go back to the lattice shown in Fig 3.4 . To simplify our discussion, let imagine that at each site there is a single elastic degree of freedom. For simplicity, let us imagine we are discussing the longitundinal displacement of an atom along a one-dimensional chain that runs in the x-direction. For the j-th atom,

$$x_j = x_j^0 + \phi_j. \tag{3.61}$$

If π_j is the conjugate momentum to x_j, then the two variables must satisfy canonical commutation relations

$$[\phi_i,\ \pi_j] = i\hbar\delta_{ij}. \tag{3.62}$$

Notice how variables at different sites are fully independent. We'll imagine that our one-dimensional lattice has N_s sites, and we shall make life easier by working with periodic boundary conditions, so that $\phi_{j+N_s} \equiv \phi_j$ and $\pi_j \equiv \pi_{j+N_s}$. Suppose nearest neighbors are connected by a "spring", in which case, the total total energy is then a sum of kinetic and potential energy

$$\hat{H} = \sum_{j=1,N_s} \left[\frac{\pi_j^2}{2m} + \frac{m\omega^2}{2} (\phi_j - \phi_{j+1})^2 \right] \tag{3.63}$$

where m is the mass of an atom.

Now the great simplifying feature of this model, is that that it possesses *translational symmetry*, so that under the translation

$$\pi_j \to \pi_{j+1}, \qquad \phi_j \to \phi_{j+1} \tag{3.64}$$

the Hamiltonian and commutation relations remain unchanged. If we shrink the size of the lattice to zero, this symmetry will become a continuous translational symmetry. The generator of these translations is the *crystal momentum* operator, which must therefore commute with the Hamiltonian. Because of this symmetry, it makes sense to transform to operators that are diagonal in momentum space, so we'll Fourier transform all fields as follows:

$$\left.\begin{array}{ll} \phi_j &= \frac{1}{\sqrt{N_s}} \sum_q e^{iqR_j} \phi_q, \\ \pi_j &= \frac{1}{\sqrt{N_s}} \sum_q e^{iqR_j} \pi_q, \end{array}\right\} \qquad R_j = ja. \tag{3.65}$$

The periodic boundary conditions, $\phi_j = \phi_{j+N_s}, \pi_j = \pi_{j+N_s}$ mean that the values of q entering in this sum must satisfy $qL = 2\pi n$, where $L = N_s a$ is the length of the chain and n is an integer, thus

$$q = \frac{2\pi}{L} n, \qquad (n \in [1, N_s]) \tag{3.66}$$

Notice that $q \in [0,\ 2\pi/a]$ defines the range of q. As in any periodic structure, the crystal momentum is only defined modulo a reciprocal lattice vector, which in this case is $2\pi/a$, so that $q + \frac{2\pi}{a} \equiv q$,

(you may verify that $(q + \frac{2\pi}{a})R_j = qR_j + 2\pi m$, which is why we restrict $n \in [1, N_s]$). The functions $\frac{1}{\sqrt{N_s}} e^{iqR_j} \equiv \langle j|q\rangle$ form a complete orthogonal basis, so that in particular

$$\sum_j \langle q'|j\rangle\langle j|q\rangle \equiv \frac{1}{N_s}\sum_j e^{i(q-q')R_j} = \langle q'|q\rangle \equiv \delta_{q,q'}. \qquad \text{orthogonality} \tag{3.67}$$

is one if $q = q'$, but zero otherwise (see exercise 3.1). This result is immensely useful, and we shall use it time and time again. Using the orthogonality relation, we can check that the inverse transformations are

$$\begin{aligned} \phi_q &= \tfrac{1}{\sqrt{N_s}}\textstyle\sum_j e^{-iqR_j}\phi_j \\ \pi_q &= \tfrac{1}{\sqrt{N_s}}\textstyle\sum_q e^{-iqR_j}\pi_j \end{aligned} \tag{3.68}$$

Notice that since ϕ_j and π_j are Hermitian operators, it follows that ${\phi^\dagger}_q = \phi_{-q}$ and ${\pi^\dagger}_q = \pi_{-q}$. Using the orthogonality, we can verify the transformed commutation relations are

$$\begin{aligned} [\phi_{-q}, \pi_{q'}] &= \frac{1}{N_s}\sum_{i,j} e^{i(qR_i - q'R_j)}\overbrace{[\phi_i, \pi_j]}^{i\hbar\delta_{ij}} \\ &= \frac{i\hbar}{N_s}\sum_j e^{i(q-q')R_j} = i\hbar\delta_{qq'} \end{aligned} \tag{3.69}$$

We shall now see that π_q and ϕ_q are quantized version of "normal co-ordinates" which bring the Hamiltonian back into the standard Harmonic oscillator form. To check that the Hamiltonian is truly diagonal in these variables we

1. expand ϕ_j and π_j in terms of their Fourier components,
2. regroup the sums so that the summation over momenta is on the outside,
3. Eliminate all but one summation over momentum by carrying out the internal sum over site variables. This will involve terms like $N_s^{-1}\sum_j e^{i(q+q')R_j} = \delta_{q+q'}$, which constrains $q' = -q$ and eliminates the sum over q'.

With a bit of practice, these steps can be carried out very quickly. In transforming the potential energy, it is useful to rewrite it in the form

$$V = \frac{m\omega^2}{2}\sum_j \phi_j(2\phi_j - \phi_{j+1} - \phi_{j-1}). \tag{3.70}$$

The term in brackets can be Fourier transformed as follows:

$$\omega^2(2\phi_j - \phi_{j+1} - \phi_{j-1}) = \frac{1}{\sqrt{N_s}}\sum_q \overbrace{\omega^2[2 - e^{iqa} - e^{-iqa}]}^{4\omega^2\sin^2(qa/2)\equiv\omega_q^2} \times \phi_q\, e^{iqR_j}$$

$$\equiv \frac{1}{\sqrt{N_s}}\sum_q \omega_q^2\,\phi_q\, e^{iqR_j}, \tag{3.71}$$

where we have defined $\omega_q^2 = 4\omega\sin^2(qa/2)$. Inserting this into (3.70), we obtain

$$\begin{aligned} V &= \frac{m}{2}\sum_{q,q'}\omega_q^2\,\phi_{-q'}\phi_q\overbrace{N_s^{-1}\sum_j e^{i(q-q')R_j}}^{\delta_{q,q'}} \\ &= \sum_q \frac{m\omega_q^2}{2}\phi_{-q}\phi_q. \end{aligned} \tag{3.72}$$

Carrying out the same procedure on the kinetic energy, we obtain

$$H = \sum_q\left(\frac{1}{2m}\pi_q\pi_{-q} + \frac{m\omega_q^2}{2}\phi_q\phi_{-q}\right) \tag{3.73}$$

which expresses the Hamiltonian in terms of "normal co-ordinates", ϕ_q and π_q. So far, all of the transformations we have preserved the ordering of the operators, so it is no surprise that the quantum and classical expressions for the Hamiltonian in terms of normal co-ordinates are formally identical.

Now before we go on, it is perhaps useful to note that at $q = 0$, $\omega_q = 0$, so that there is no contribution to the potential energy from the $q = 0$ mode, which corresponds to a uniform translation of the entire system. To separate the uniform motion from the oscillatory modes, it is useful to split the $q = 0$ part of the Hamiltonian off from the remainder,

$$H = \overbrace{\frac{1}{2m}\pi_0^2}^{H_{CM}} + \sum_{q\neq 0}\left(\frac{1}{2m}\pi_q\pi_{-q} + \frac{m\omega_q^2}{2}\phi_q\phi_{-q}\right)$$

where the first term is just the center of mass energy.

The next step merely repeats the procedure carried out for the single harmonic oscillator. We define a set of conjugate creation and annihilation operators

$$\left.\begin{aligned} a_q &= \sqrt{\tfrac{m\omega_q}{2\hbar}}(\phi_q + \tfrac{i}{m\omega_q}\pi_q) \\ {a^\dagger}_q &= \sqrt{\tfrac{m\omega_q}{2\hbar}}(\phi_{-q} - \tfrac{i}{m\omega_q}\pi_{-q}) \end{aligned}\right\} \qquad [a_q,\ {a^\dagger}_{q'}] = \tfrac{-i}{2\hbar}\Big[[\phi_q, \pi_{-q'}] - [\pi_q, \phi_{-q'}]\Big] = \delta_{q,q'} \tag{3.74}$$

Note that the second expression for ${a^\dagger}_q$ is obtained by taking the complex conjugate of a_q, and remembering that ${\phi^\dagger}_q = \phi_{-q}$ and ${\pi^\dagger}_q = \pi_{-q}$, since the underlying fields are real.

The inversion of these expressions is

$$\left.\begin{aligned} \pi_q &= -i\sqrt{\tfrac{m\omega_q\hbar}{2}}(a_q - {a^\dagger}_{-q}) \\ \phi_a &= \sqrt{\tfrac{\hbar}{2m\omega_q}}(a_q + {a^\dagger}_{-q}) \end{aligned}\right\} \tag{3.75}$$

Notice how the Fourier component of the field at wavevector q either destroys a phonon of momentum q or creates a phonon of momentum $-q$. Both have reduce the total momentum by q.

From these expressions, it follows that

$$\begin{aligned}\pi_q\pi_{-q} &= \frac{m\omega_q\hbar}{2}(a^\dagger{}_{-q}a_{-q} + a_q a^\dagger{}_q - a^\dagger{}_{-q}a^\dagger{}_q - a_q a_{-q}) \\ \phi_q\phi_{-q} &= \frac{\hbar}{2m\omega_q}(a^\dagger{}_{-q}a_{-q} + a_q a^\dagger{}_q + a^\dagger{}_{-q}a^\dagger{}_q + a_q a_{-q})\end{aligned} \tag{3.76}$$

Adding the two terms inside the Hamiltonian then gives

$$H = H_{CM} + \frac{1}{2}\sum_{q\neq 0}\hbar\omega_q(a^\dagger{}_q a_q + a_q a^\dagger{}_q), \tag{3.77}$$

or using the commutation relations,

$$H = H_{CM} + \sum_{q\neq 0}\hbar\omega_q(a^\dagger{}_q a_q + \frac{1}{2}) \tag{3.78}$$

Since each set of a_q and $a^\dagger{}_q$ obey canonical commutation relations, we can immediately identify $n_q = a^\dagger{}_q a_q$ as the number operator for quanta in the q-th momentum state. Remarkably, the system of coupled oscillators can be reduced to a sum of independent Harmonic oscillators, with characteristic frequency ω_q, energy $\hbar\omega_q$ and momentum q. Each normal mode of the original classical system corresponds to particular phonon excitation.

We can immediately generalize all of our results from a single Harmonic oscillator. For example, the general state of the system will now be an eigenstate of the phonon occupancies,

$$|\Psi\rangle = |n_{q_1},\ n_{q_2}\ldots n_{q_N}\rangle = \prod_{\otimes}|n_{q_i}\rangle = \left[\prod_i \frac{(a^\dagger{}_{q_i})^{n_{q_i}}}{\sqrt{n_{q_i}!}}\right]|0\rangle \tag{3.79}$$

where the vacuum is the unique state that is annihilated by all of the a_q. In this state, the occupation numbers n_q are diagonal, so this is an energy eigenstate with energy

$$E = E_o + \sum_q n_q\hbar\omega_q \tag{3.80}$$

where $E_o = \frac{1}{2}\sum_q \hbar\omega_q$ is the zero-point energy.

Remarks

- The quantized displacements of a crystal are called phonons. Quantized fluctuations of magnetization in a magnet are "magnons".
- We can easily transform to a Heisenberg representation, whereapon $a_q(t) = a_q e^{-i\omega_q t}$.

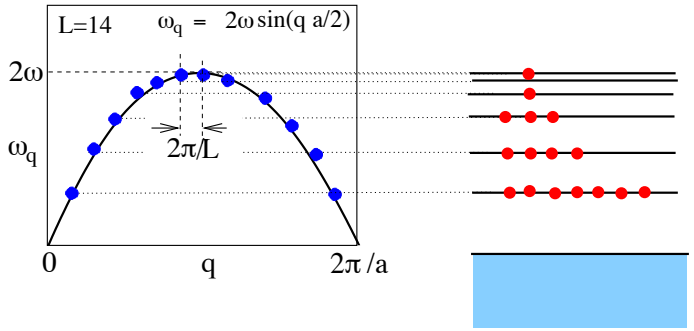

Figure 3.6: Illustrating the excitation picture for a chain of coupled oscillators, length L=14.

- We can expand the local field entirely in terms of phonons. Using (3.75), we obtain

$$\begin{aligned}\phi_j(t) &= \frac{1}{\sqrt{N_s}}\sum_q \phi_q e^{iqR_j} \\ &= \phi_{CM}(t) + \frac{1}{\sqrt{N_s}}\sum_{q\neq 0}\sqrt{\frac{\hbar}{2m\omega_q}}\left[a_q(t) + a^\dagger{}_{-q}(t)\right]e^{iqR_j}.\end{aligned} \tag{3.81}$$

  where $\phi_{CM} = \frac{1}{N_s}\sum_j \phi_j$ is the center of mass displacement.

- The transverse displacements of the atoms can be readily included by simply upgrading the displacement and momentum ϕ_j and π_j to vectors. For "springs", the energies associated with transverse and longitudinal displacements are not the same because the stiffness associated with transverse displacements depends on the tension. Nevertheless, the Hamiltonian has an identical form for the one longitudinal and two transverse modes, provided one inserts a different stiffness for the transverse modes. The initial Hamiltonian is then simply a sum over three degenerate polarizations $\lambda \in [1, 3]$

$$\hat{H} = \sum_{\lambda=1,3}\sum_{j=1,N_s}\left[\frac{\pi^2_{j\lambda}}{2m} + \frac{m\omega^2_\lambda}{2}(\phi_{j\lambda} - \phi_{j+1\lambda})^2\right] \tag{3.82}$$

  where $\omega^2_1 = \omega^2$ for the longitudinal mode, and $\omega^2_{2,3} = T/a$, where T is the tension in the spring, for the two transverse modes. By applying the same procedure to all three modes, the final Hamiltonian then becomes

$$H = \sum_{\lambda=1,3}\sum_q \hbar\omega_{q\lambda}(a^\dagger{}_{q\lambda}a_{q\lambda} + \frac{1}{2}).$$

where $\omega_{q\lambda} = 2\omega_\lambda sin(qa/2)$. Of course, in more realistic crystal structures, the energies of the three modes will no longer be degenerate.

- We can generalize all of this discussion to a 2 or 3 dimensional square lattice, by noting that the orthogonality relation becomes

$$N_s^{-1}\sum_j e^{-i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{R}_j} = \delta_{\mathbf{q}-\mathbf{q}'} \tag{3.83}$$

where now,

$$\mathbf{q} = \frac{2\pi}{L}(i_i, i_2 \ldots i_D) \tag{3.84}$$

and $\mathbf{R_j}$ is a site on the lattice. The general form for the potential energy is slightly more complicated, but one can still cast the final Hamiltonian in terms of a sum over longitudinal and transverse modes.

- The zero-point energy $E_o = \frac{1}{2}\sum_q \hbar\omega_q$ is very important in $He-4$ and $He-3$ crystals, where the lightness of the atoms gives rise to such large phonon frequencies that the crystalline phase is unstable and melts at ambient pressure under the influence of quantum zero point motion. The resulting "quantum fluids" exhibit the remarkable property of superfluidity.

3.5 The Thermodynamic Limit

In the last section, we examined a system of coupled oscillators on a finite lattice. By restricting a system to a finite lattice, we impose a restriction on the *maximium* wavelength, and hence, the excitation spectrum. This is known as an "infra-red" cut-off. When we take $L \to \infty$, the allowed momentum states become closer and closer together, and we now have a continuum in momentum space.

What happens to the various momentum summations in the thermodynamic limit, $L \to \infty$? When the allowed momenta become arbitrarily close together, the discrete summations over momentum must be replaced by continuous integrals. For each dimension, the increment in momentum appearing inside the discrete summations is

$$\Delta q = \frac{2\pi}{L} \tag{3.85}$$

so that $L\frac{\Delta q}{2\pi} = 1$. Thus in one dimension, the summation over the discrete values of q can be formally rewritten as

$$\sum_{q_j}\{\ldots\} = L\sum_{q_j}\frac{\Delta q}{2\pi}\{\ldots\} \tag{3.86}$$

where $q_j = 2\pi\frac{j}{L}$, and $j \in [1, N_s]$. When we take $L \to \infty$, q becomes a continuous variable $q \in [0, 2\pi/a]$, where $a = L/N_s$ is the lattice spacing, so that the summation can now be replaced by a continuous integral:

$$\sum_q\{\ldots\} \to L\int_0^{2\pi/a}\frac{dq}{2\pi}\{\ldots\} \tag{3.87}$$

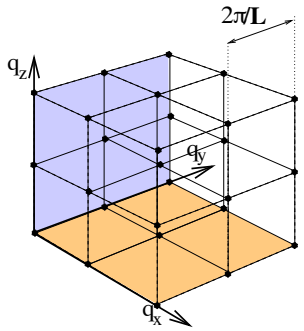

Figure 3.7: Illustrating the grid of allowed momenta for a three-dimensional crystal of dimensions L^3. In the limit $L \to \infty$, the grid becomes a continuum, with $(L/2\pi)^3$ points per unit volume of momentum space.

Similarly, in in D-dimensions, we can regard the D-dimensional sum over momentum as a sum over tiny hypercubes, each of volume

$$(\Delta q)^D = \frac{(2\pi)^D}{L^D} \tag{3.88}$$

so that $L^D\frac{(\Delta q)^D}{(2\pi)^D} = 1$ and

$$\sum_q\{\ldots\} = L^D\sum_q\frac{(\Delta q)^D}{(2\pi)^D}\{\ldots\} \to L^D\int_{0<q_i<2\pi/a}\frac{d^Dq}{(2\pi)^D}\{\ldots\} \tag{3.89}$$

where the integral is over a hypercube in momentum space, with sides of length $2\pi/a$.

Once the momentum sums become continuous, we need to change the normalization of our states. By convention, we now normalize our plane wave basis per unit volume, writing

$$\langle\mathbf{x}|\mathbf{k}\rangle \to e^{i\mathbf{k}\cdot\mathbf{x}} \tag{3.90}$$

In a finite volume, this means that the orthogonality condition on these plane waves is

$$\langle\mathbf{k}'|\mathbf{k}\rangle = \int d^Dx e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} = L^D\delta_{\mathbf{k}-\mathbf{k}'}, \tag{3.91}$$

where $\delta_{\mathbf{k}-\mathbf{k}'}$ is the discrete delta function on the grid of allowed wavevectors. In the thermodynamic limit, this becomes

$$\int d^Dx e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} = (2\pi)^D\delta^D(\mathbf{k}-\mathbf{k}') \tag{3.92}$$

so that the continuum limit of the discrete delta-function is given by

$$L^D \delta_{\mathbf{k}\mathbf{k}'} \longrightarrow (2\pi)^D \delta^D(\mathbf{k}-\mathbf{k}') \tag{3.93}$$

Example 4. *Re-express the Hamiltonian $\hat{H}$ of a simplified three-dimensional Harmonic crystal in terms of phonon number operators and calculate the zero-point energy, where*

$$H = \sum_j \frac{\pi_j^2}{2m} + \sum_{j,\mathbf{a}=(\hat{x},\hat{y},\hat{z})} \frac{m\omega_o^2}{2}(\Phi_j - \Phi_{j+\mathbf{a}})^2 \tag{3.94}$$

where $\phi_j \equiv \phi(x_j)$ and $\pi_j \equiv \pi(x_j)$ denote canonically conjugate (scalar) displacement, and momenta at site j, and $\hat{a} = (\hat{x},\hat{y},\hat{z})$ denotes the unit vector separating nearest neigbor atoms.

Solution First we must Fourier transform the co-ordinates and the Harmonic potential. The potential can be re-written as

$$\hat{V} = \frac{1}{2}\sum_{i,j} V_{i-j}\phi_i\phi_j \tag{3.95}$$

where

$$V_{\mathbf{R}} = m\omega_o^2 \sum_{\mathbf{a}=(\hat{x},\hat{y},\hat{z})} (2\delta_{\mathbf{R}} - \delta_{\mathbf{R}-\mathbf{a}} - \delta_{\mathbf{R}+\mathbf{a}}) \tag{3.96}$$

The Fourier transform of this expression is

$$\begin{aligned} V_{\mathbf{q}} &= \sum_{\mathbf{R}} V_{\mathbf{R}} e^{-i\mathbf{q}\cdot\mathbf{R}} \\ &= m\omega_o^2 \sum_{\mathbf{a}=(\hat{x},\hat{y},\hat{z})} (2 - e^{-i\mathbf{q}\cdot\mathbf{a}} - e^{i\mathbf{q}\cdot\mathbf{a}}) \\ &= m\omega_o^2 \sum_{l=x,y,z} [2 - \cos(q_l a)] \end{aligned} \tag{3.97}$$

so that writing $V_{\mathbf{q}} = m(\omega_{\mathbf{q}})^2$, it follows that the normal mode frequency are given by

$$\omega_{\mathbf{q}} = 2\omega_o[\sin^2(q_x a/2) + \sin^2(q_y a/2) + \sin^2(q_z a/2)]^{\frac{1}{2}} \tag{3.98}$$

Fourier transforming the fields

$$\begin{aligned} \phi_j &= \frac{1}{\sqrt{N_s}}\sum_{\mathbf{q}} \phi_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}} \\ \pi_j &= \frac{1}{\sqrt{N_s}}\sum_{\mathbf{q}} \pi_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}} \end{aligned} \tag{3.99}$$

where $\mathbf{q} = \frac{2\pi}{L}(i,j,k)$ are the discrete momenta of a cubic crystal of volume L^3, with periodic boundary conditions, we find

$$H = \sum_{\mathbf{q}} \Big[\frac{\pi_{\mathbf{q}}\pi_{-\mathbf{q}}}{2m} + \frac{m\omega_{\mathbf{q}}^2}{2}\phi_{\mathbf{q}}\phi_{-\mathbf{q}} \Big] \tag{3.100}$$

Defining the creation and annihilation operator

$$b_{\mathbf{q}} = \sqrt{\frac{m\omega_{\mathbf{q}}}{2\hbar}}(\phi_{\mathbf{q}} + \frac{i}{m\omega_{\mathbf{q}}}\pi_{\mathbf{q}}), \qquad b^\dagger{}_{\mathbf{q}} = \sqrt{\frac{m\omega_{\mathbf{q}}}{2\hbar}}(\phi_{-\mathbf{q}} - \frac{i}{m\omega_{\mathbf{q}}}\pi_{-\mathbf{q}}), \tag{3.101}$$

we reduce the Hamiltonian to its standard form

$$H = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}}(\hat{n}_{\mathbf{q}} + \frac{1}{2}) \tag{3.102}$$

where $\hat{n}_{\mathbf{q}} = b^\dagger{}_{\mathbf{q}} b_{\mathbf{q}}$ is the phonon number operator.
In the ground-state, $n_{\mathbf{q}} = 0$, so that the zero-point energy is

$$E_o = \sum_{\mathbf{q}} \frac{\hbar\omega_{\mathbf{q}}}{2} \longrightarrow V\int \frac{d^3q}{(2\pi)^3}\frac{\hbar\omega_{\mathbf{q}}}{2} \tag{3.103}$$

where $V = L^3$. Substituting for $\omega_{\mathbf{q}}$, we obtain

$$\begin{aligned} E_o &= V\prod_{l=1,3}\int_0^{2\pi/a}\frac{dq_l}{2\pi}\hbar\omega_o\sqrt{\sum_{l=1,3}\sin^2(q_l a/2)} \\ &= N_s\hbar\omega_o I_3 \end{aligned} \tag{3.104}$$

where

$$I_3 = \int_{0<u_1,u_2,u_3<\pi}\frac{d^3u}{\pi^3}\sqrt{\sum_{l=1,3}\sin^2(u_l)} = 1.19 \tag{3.105}$$

and N_s is the number of sites.

Remarks

- The zero point energy per unit cell of the crystal is $\hbar\omega_o(I_3/\pi^3)$, a finite number.
- Were we to take the "continuum limit", taking the lattice separation to zero, the zero-point energy would diverge, due to the profusion of ultraviolet modes.

3.6 Continuum Limit

In contrast to the thermodynamic limit, when we take the continuum limit we remove the discrete character of the problem, allowing fluctuations of arbitrarily small wavelength, and hence arbitrarily large energy. For a discrete system with periodic boundary conditions, the momentum in any one direction can not exceed $2\pi/a$. By taking a to zero, we remove the ultra-violet cut-off in momentum.

As a simple example, we shall consider a one-dimensional string. The important lesson that we shall learn, is that both the discrete model, and the continuum model have the same long-wavelength physics. Their behavior will only differ on very short distances, at high frequencies and short times.

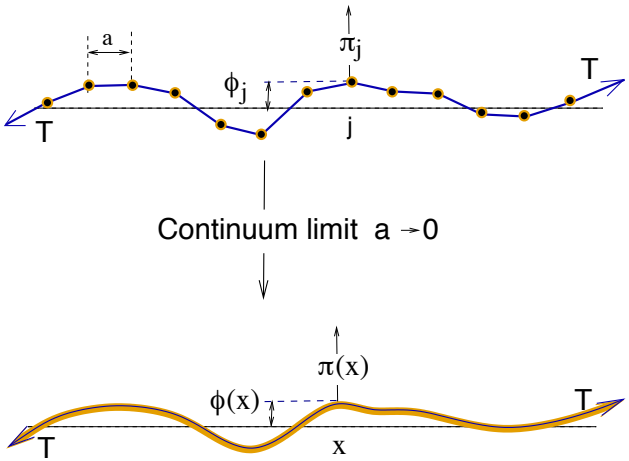

Figure 3.8: Illustrating a (a) discrete and a (b) continuous string. By taking the length between units in the string to zero, maintaining the density per unit length and the tension, we arrive at the continuum limit.

This is a very simple example of the concept of renormalization. Provided we are interested in low energy properties, the details of the string at short-distances- whether it is discrete, or continuous don't matter.

Of course, in many respects, the continuum model is more satisfying and elegant. We shall see however, that we always have to be careful in going to the continuum limit, because this introduces quantum fluctuations on arbitrarily short length scales. These fluctuations don't affect the low energy excitations, but they do mean that the zero-point fluctuations of the field become arbitrarily large.

Let us start out with a discrete string, as shown in fig 3.8. For small displacements, the Hamiltonian for this discrete string is identical to that of the last section, as we can see by the following argument. If a string is made up of point particles of mass m, separated by a distance a, with a tensile force T acting between them, then for small transverse displacements ϕ_j, the link between the j th and $j+1$th particle is expanded by an amount $\Delta s_j = (\phi_j - \phi_{j+1})^2/2a$, raising the potential

energy by an amount $T\Delta s_j$. The Hamiltonian is then

$$\hat{H} = \sum_{j=1,N_s}\left[\frac{\pi_j^2}{2m} + \frac{T}{2a}(\phi_j - \phi_{j+1})^2\right] \tag{3.106}$$

which reverts to (3.63) with the replacement $T/a \to m\omega^2$.

To take the continuum limit, we let $a \to 0$, preserving $\rho = m/a$. In this limit, we may replace

$$\begin{aligned} a\sum_j &\to \int dx, \\ \frac{(\phi_j - \phi_{j+1})^2}{a^2} &\to (\nabla_x\phi(x))^2, \end{aligned} \tag{3.107}$$

Making the replacement

$$\pi_j/a \to \pi(x_j) \tag{3.108}$$

we obtain

$$H = \int dx\left[\frac{T}{2}(\nabla_x\phi)^2 + \frac{1}{2\rho}\pi(x)^2\right] \tag{3.109}$$

On the discrete lattice, the commutation relations

$$[\phi(x_i), \pi(x_j)] = i\hbar\tilde{\delta}(x_i - x_j), \tag{3.110}$$

where $\tilde{\delta}(x_i - x_j) = a^{-1}\delta_{ij}$. In the limit $a \to 0$, $\tilde{\delta}(x_i - x_j)$ behaves as a Dirac delta function, so that in this limit,

$$[\phi(x), \tilde{\pi}(y)] = i\hbar\delta(x - y) \tag{3.111}$$

We now make the jump to Fourier space, writing

$$\phi(x) = \int \frac{dq}{2\pi}\phi_q e^{iqx}e^{-\epsilon|q|/2} \tag{3.112}$$

with a similar relation between $\pi(x)$ and π_q. In the continuum limit, q is no longer bounded by the cut-off $2\pi/a$. To control the wild fluctuations that arise at high momentum we still need some kind of cut-off, and this is why we introduce the small exponential convergence factor into the inverse Fourier transform. Now it is just a question of repeating the same steps of the last section, but for the continuous fields ϕ_q and π_q. We may confirm that in the canonical commutation relation, we must now replace $\langle q|q'\rangle = \delta_{qq'}$ by $\langle q|q'\rangle = 2\pi\delta(q - q')$, so that

$$[\phi_q, \pi_{-q'}] = i\hbar 2\pi\delta(q - q') \tag{3.113}$$

When we transform the Hamiltonian, we obtain

$$H = \int \frac{dq}{2\pi}\left[\frac{\pi_{\mathbf{q}}\pi_{-\mathbf{q}}}{2\rho} + \frac{\rho\omega_{\mathbf{q}}^2}{2}\phi_{\mathbf{q}}\phi_{-\mathbf{q}}\right]e^{-\epsilon|q|} \tag{3.114}$$

where now $\omega_q = c|q|$, and $c = \sqrt{T/\rho}$ is the velocity of the phonons. Notice how this has almost exactly the same form as the the discrete lattice. Defining the creation and annihilation operator by the relations

$$\begin{aligned}\phi_q &= \sqrt{\frac{\hbar}{2\rho\omega_q}}[a_q + a^\dagger{}_{-q}] \\ \pi_q &= -i\sqrt{\frac{\hbar\rho\omega_q}{2}}[a_q - a^\dagger{}_{-q}]\end{aligned} \tag{3.115}$$

we find that the creation and annihilation operators satisfy

$$[a_q, a^\dagger{}_{q'}] = 2\pi\delta(q-q'). \tag{3.116}$$

We may now rewrite the Hamiltonian as

$$H = \int_{-\infty}^{\infty}\frac{dq}{2\pi}\frac{\hbar\omega_{\mathbf{q}}}{2}(a^\dagger{}_q a_q + a_{-q}a^\dagger{}_{-q})e^{-\epsilon|q|} \tag{3.117}$$

If we re-order the Boson operators, we obtain

$$H = \int_{\infty}^{\infty}\frac{dq}{2\pi}\hbar\omega_{\mathbf{q}}(a^\dagger{}_q a_q + \overbrace{2\pi\delta(0)}^{\text{“}L\text{”}}\frac{1}{2})e^{-|\epsilon q|/2} \tag{3.118}$$

The first terms corresponds to the excitations of string, and we recognize the last term as the zero-point energy of the string. Had we been less ambitious, and started out on a finite, but long lattice , the term $2\,\pi\delta(0)$ would be replaced by L, which is merely the statement that the zero-point energy scales with the length,

$$E_{ZP} = L\int\frac{dq}{2\pi}\hbar c|q|e^{-\epsilon|q|} = \frac{L\hbar c}{2\pi\epsilon^2} \tag{3.119}$$

is the total zero-point energy. Once we remove the momentum cut-off, the momentum sum is unbounded and the zero-point energy per unit length becomes infinite in the continuum limit. It often proves convenient to remove this nasty infinity by introducing the concept of *“normal ordering”*. If we take any operator A, then we denote its normal ordered count-part by the symbol $:A:$. The operator $:A:$ is the same as A, excepting that all the creation operators have been ordered to the left of all of the annihilation operators. All commutators associated with the ordering are neglected, so that the normal ordered Hamiltonian is

$$:H: = \int_{-\infty}^{\infty}\frac{dq}{2\pi}\hbar\omega_q a^\dagger{}_q a_q, \qquad (\omega_q = c|q|) \tag{3.120}$$

measures the excitation energy above the ground-state.

Finally, let us look at the field correlations in the continuum string. The fields in co-ordinate space are given by

$$\phi(x,t) = \int\frac{dq}{2\pi}\sqrt{\frac{\hbar}{2\rho\omega_q}}[a_q(t) + a_{-q}(t)]e^{iqx}e^{-\epsilon|q|/2} \tag{3.121}$$

where, as in the case of the Harmonic oscillator

$$a_q(t) = a_q e^{-i\omega_q t}, \qquad a^\dagger{}_q(t) = a_q e^{i\omega_q t}, \tag{3.122}$$

Note:

- The generalization of the “quantum string” two higher dimensions is written

$$\begin{aligned}H &= \int d^dx\left[\frac{T}{2}(\nabla\phi)^2 + \frac{1}{2\rho}\pi(x)^2\right] \\ [\phi(x),\pi(y)] &= i\hbar\delta^d(x-y).\end{aligned} \tag{3.123}$$

  Sometimes, it is useful to rescale $\phi(x) \to \phi(x)/\sqrt{\rho}$, $\pi(x) \to \pi(x)\sqrt{\rho}$, so that

$$\begin{aligned}H &= \frac{1}{2}\int d^dx\left[(c\nabla\phi)^2 + \pi(x)^2\right] \\ [\phi(x),\tilde{\pi}(y)] &= i\hbar\delta^d(x-y).\end{aligned} \tag{3.124}$$

  In two dimensions, this describes a fluctuating quantum membrane.

- In particle physics, the “massive” version of the above model, written as

$$H = \frac{1}{2}\int d^dx\left[\phi\left(-c^2\nabla^2 + \left(\frac{mc^2}{\hbar}\right)^2\right)\phi + \pi^2\right] \tag{3.125}$$

  where c is the speed of light, is called the “Klein-Gordon Hamiltonian”. In this model, the elementary quanta have energy $E_q = \sqrt{(\hbar cq)^2 + (mc^2)^2}$.

Example 5. *Calculate the the equal-time ground-state correlation function*

$$S(x) = \frac{1}{2}\langle 0|(\phi(x) - \phi(0))^2|0\rangle. \tag{3.126}$$

for a one-dimensional string.

Solution: Let us begin by rewriting

$$S(x) = \langle 0|(\phi(0)^2 - \phi(x)\phi(0))|0\rangle \tag{3.127}$$

where we have used translational invariance to replace the expectation value of $\phi(x)^2$ by the expectation value of $\phi(0)^2$. When we expand $\phi(x)$ and $\phi(0)$ in terms of creation and annihilation operators, only the terms of the form $\langle 0|a_q a^\dagger{}_{-q'}|o\rangle = \langle 0|[a_q, a^\dagger{}_{-q'}]|o\rangle = (2\pi)\delta(q-q')$ will survive. Let us write this out explicitly:

$$S(x) = \int\frac{dqdq'}{(2\pi)^2}\frac{\hbar}{2\rho c\sqrt{|q||q'|}}\langle 0|[a_q + a^\dagger{}_{-q}][a_{-q'} + a^\dagger{}_{q'}]|0\rangle(e^{iqx} - 1)e^{-|q|\epsilon}$$

$$= \frac{\hbar}{2\rho c}\int \frac{dq}{2\pi} e^{-|q|\epsilon}\Big(\frac{1-e^{iqx}}{|q|}\Big)$$
$$= \Big(\frac{\hbar}{\rho c}\Big)\Big[\frac{1}{4\pi}\ln(\frac{\epsilon^2+x^2}{\epsilon^2})\Big] \quad (3.128)$$

where to obtain the last step, we first calculate

$$\frac{dS}{dx} = \frac{\hbar}{\rho c}\mathrm{Im}\int_0^\infty \frac{dq}{\pi} e^{-q(\epsilon - ix)} = \Big(\frac{\hbar}{2\pi\rho c}\Big)\mathrm{Im}\frac{1}{\epsilon - ix} \quad (3.129)$$

and then integrate the answer on x, noting that $S(0) = 0$.

Remarks

- Note that at small distances the fluctuations in the string displacement grow as $\ln(|x|)$. This is because the number of short-wavelength fluctuations is unbounded.
- Note also that we could have obtained this result by working with a discrete string, and taking $a \to 0$ at the end of the calculation. Had we done this, we would have found that

$$S(x) = \frac{\hbar}{2m}\sum_q \Big(\frac{1-e^{iqx}}{\omega_q}\Big) \quad (3.130)$$

  which has the same long-wavelength behavior.
- Had we repeated this calculation in D dimensions, the integral over q becomes a d-dimensional integral. In this case,

$$S(x) \sim \int d^D q\Big(\frac{1-e^{iqx}}{|q|}\Big) \sim \frac{1}{x^{D-1}} \quad (3.131)$$

  In higher dimensions, the phase space for number of short-wavelength fluctuations grows as q^D, which leads to stronger fluctuations at short-distances.

3.7 Exercises

1. Consdier the orthogonality relation in equation (3.67)

$$\sum_j \langle q_m|j\rangle\langle j|q_n\rangle \equiv \frac{1}{N_s}\sum_j e^{i(q_n - q_m)R_j} = \delta_{nm}, \quad (3.132)$$

where $q_n = n\frac{2\pi}{L}$, $q = n\frac{2\pi}{L} = n\frac{2\pi}{N_s a}$ are the discrete wavevectors, $N_s = L/a$ is the number of sites in the chain and a is the lattice spacing. By substituting $R_j = ja$ and treating this expression as a geometric series, show that

$$\sum_j \langle q_m|j\rangle\langle j|q_n\rangle \equiv \frac{1}{N_s}\sum_j e^{i(q_n - q_m)R_j} = \frac{1}{N_s}\frac{\sin[\pi(n-m)]}{\sin[\frac{\pi}{N_s}(n-m)]} \equiv \delta_{nm}$$

thereby proving orthogonality.

2. For the Harmonic oscillator $H = \hbar\omega[a^\dagger a + \frac{1}{2}]$, we know that

$$\langle \hat{n}\rangle = n(\omega) = \frac{1}{e^{\beta\hbar\omega} - 1}, \quad (3.133)$$

where $\beta = 1/(k_B T)$ and $\hat{n} = a^\dagger a$ is the number operator. In the ground-state, using the equations of motion for the creation and annihilation operators, we showed that the zero-point fluctuations in position were described by the correlation function

$$\frac{1}{2}\langle\{x(t),\ x(0)\}\rangle = \frac{\hbar}{2m\omega}\cos\omega t. \quad (3.134)$$

Generalize this result to finite temperatures. You should find that there are two terms in the correlation function. *Please* give them a physical interpretation.

3. (a) Show that if a is a canonical bose operator, the canonical transformation

$$b = ua + va^\dagger,$$
$$b^\dagger = ua^\dagger + va, \quad (3.135)$$

(where u and v are real), preserves the canonical commutation relations, provided $u^2 - v^2 = 1$.

(b) Using the results of (a), diagonalize the Hamiltonian

$$H = \omega(a^\dagger a + \frac{1}{2}) + \frac{1}{2}\Delta(a^\dagger a^\dagger + aa), \quad (3.136)$$

by transforming it into the form $H = \tilde{\omega}(b^\dagger b + \frac{1}{2})$. Find $\tilde{\omega}$, u and v in terms of ω and Δ. What happens when $\Delta = \omega$?

(c) The Hamiltonian in (b) has a boson pairing term. Show that the ground-state of H can be written as coherent condensate of paired bosons, given by

$$|\tilde{0}\rangle = e^{-\alpha(a^\dagger a^\dagger)}|0\rangle.$$

Calculate the value of α in terms of u and v. (*Hint: $|\tilde{0}\rangle$ is the vacuum for b, i.e $b|\tilde{0}\rangle = (ua + va^\dagger)|\tilde{0}\rangle = 0$. Calculate the commutator of $[a, e^{-\alpha a^\dagger a^\dagger}]$ by expanding the exponential as a power series. Find a value of α that guarantees that b annihilates the vacuum $|\tilde{0}\rangle$.)*

4. (Harder) Find the classical normal mode frequencies and normal co-ordinates for the one dimensional chain with Hamiltonian

$$H = \sum_j \Big[\frac{p_j^2}{2m_j} + \frac{k}{2}(\phi_j - \phi_{j-1})^2\Big] \quad (3.137)$$

where at even sites $m_{2j} = m$ and at odd sites $m_{2j+1} = M$. Please sketch the dispersion curves.

(ii) What is the gap in the excitation spectrum?

(iii)Write the diagonalized Hamiltonian in second quantized form and discuss how you might arrive at your final answer. You will now need two types of creation operator.

5. (Harder) According to the "Lindeman" criterion, a crystal melts when the rms displacement of its atoms exceeds a third of the average separation of the atoms. Consider a three dimensional crystal with separation a, atoms of mass m and a nearest neigbor quadratic interaction $V = \frac{m\omega^2}{2}(\vec{\Phi}_{\mathbf{R}} - \vec{\Phi}_{\mathbf{R}+\mathbf{a}})^2$.

   (i) Estimate the amplitude of zero point fluctuations using the uncertainty principle, to show that if

   $$\frac{\hbar}{m\omega a^2} > \zeta_c \tag{3.138}$$

   where ζ_c is a dimensionless number of order one, the crystal will be unstable, even at absolute zero, and will melt due to zero-point fluctuations. (Hint... what would the answer be for a simple harmonic oscillator?)

   (ii) Calculate ζ_c in the above model. If you like, to start out, imagine that the atoms only move in one direction, so that Φ is a scalar displacement at the site with equilibrium position $\mathbf{R}$. Calculate the rms zero-point displacement of an atom $\sqrt{\langle 0|\Phi(x)^2|0\rangle}$. Now generalize your result to take account of the fluctuations in three orthogonal directions.

   (iii)Suppose $\hbar\omega/k_B = 300K$, and the atom is a Helium atom. Assuming that ω is independent of atom separation a, estimate the critical atomic separation a_c at which the solid becomes unstable to quantum fluctuations. Note that in practice ω is dependent on a, and rises rapidly at short distances, with $\omega \sim a^{-\alpha}$, where $\alpha > 2$. Is the solid stable for $a < a_c$ or for $a > a_c$?

6. (Harder) Find the transformation that diagonalizes the Hamiltonian

   $$H = \sum_j \left\{ J_1(a^\dagger_{i+1}a_i + H.c) + J_2(a^\dagger_{i+1}a^\dagger_i + H.c) \right\} \tag{3.139}$$

   where the ith site is located at $R_j = aj$. You may find it helpful to (i) transform to momentum space, writing $a_j = \frac{1}{N^{1/2}}\sum_q e^{iqR_j}a_q$ and (ii) carrying out a canonical transformation of the form $b_q = u_q a_q + v_q a^\dagger_{-q}$, where $u^2 - v^2 = 1$. What happens when $J_1 = J_2$?

7. (Harder) This problem sketches the proof that the displacement of the quantum Harmonic oscillator, originally in its ground-state (in the distant past), is given by

   $$\langle x(t)\rangle = \int_0^\infty R(t-t')f(t')dt', \tag{3.140}$$

   where

   $$R(t-t') = \frac{i}{\hbar}\langle 0|[x(t), x(t')]|0\rangle \tag{3.141}$$

   is the "response function" and $x(t)$ is the position operator in the Heisenberg representation of H_0. A more detailed discussion can be found in chapter 10.

   An applied force $f(t)$ introduces an additional forcing term to the harmonic oscillator Hamiltonian

   $$\hat{H}(t) = H_0 + V(t) = \hat{H}_0 - f(t)\hat{x}, \tag{3.142}$$

   where $H_0 = \hbar\omega(a^\dagger a + \frac{1}{2})$ is the unperturbed Hamiltonian. To compute the displacement of the Harmonic oscillator, it is convenient to work in the "interaction representation", which is the Heisenberg representation for H_0. In this representation, the time-evolution of the wavefunction is due to the force term. The wavefunction of the harmonic oscillator in the interation representation $|\psi_I(t)\rangle$ is related to the Schrodinger state $|\psi_S(t)\rangle$ by the relation $|\psi_I(t)\rangle = e^{iH_0t/\hbar}|\psi_S(t)\rangle$.

   (a) By using the equation of motion for the Schrodinger state $i\hbar\partial_t|\psi_S(t)\rangle = (H_0 + V(t))|\psi_S(t)\rangle$, show that the time evolution of the wavefunction in the interaction representation is

   $$i\hbar\partial_t|\psi_I(t)\rangle = V_I(t)|\psi_I(t)\rangle = -f(t)\hat{x}(t)|\psi_I(t)\rangle, \tag{3.143}$$

   where $V_I(t) = e^{iH_0t/\hbar}\hat{V}(t)e^{-iH_0t/\hbar} = -x(t)f(t)$ is the force term in the interaction representation.

   (b) Show that if $|\psi(t)\rangle = |0\rangle$ at $t = -\infty$, then the leading order solution to the above equation of motion is then

   $$|\psi_I(t)\rangle = |0\rangle + \frac{i}{\hbar}\int_{-\infty}^t dt' f(t')\hat{x}(t')|0\rangle + O(f^2), \tag{3.144}$$

   so that

   $$\langle\psi_I(t)| = \langle 0| - \frac{i}{\hbar}\int_{-\infty}^t dt' f(t')\langle 0|\hat{x}(t') + O(f^2). \tag{3.145}$$

   (c) Using the results just derived expand the expectation value $\langle\psi_I(t)|x(t)|\psi_I(t)\rangle$ to linear order in f, obtaining the above cited result.

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Chapter 4

Conserved Particles

The method we have just examined is fine for "collective excitations" of a medium, but it does not make it self-evident how we should proceed for systems of conserved particles, such as a gas of Helium-4 atoms, or an electron gas inside a metal. Now we shall return to discuss conserved particles.

First quantized quantum mechanics *can* deal with many body physics, through the introduction of a many particle wavefunction. This is the approach favored in fields such as quantum chemistry, where the number of electrons is large, but not macroscopic. The quantum chemistry approach revolves around the many-body wavefunction. For N particles, this a function of $3N$ variables and N spins. The Hamiltonian is then an operator expressed in terms of these co-ordinates:

$$\begin{aligned} \psi &\rightarrow \psi(x_1, x_2 \ldots x_N, t) \\ H &\rightarrow \sum_j \left[-\frac{\hbar^2}{2m}\nabla_j^2 + U(x_j) \right] + \frac{1}{2}\sum_{i<j} V(x_i - x_j) \end{aligned} \tag{4.1}$$

With a few famous exceptions this method is cumbersome, and ill-suited to macroscopically large systems. The most notable exceptions occur in low dimensional problems, where wavefunctions of macroscopically large ensembles of interacting particles have been obtained. Examples include

- Bethe Ansatz solutions to interacting one dimensional, and impurity problems[1, 2, 3, 4].
- Laughlin's wavefunction for interacting electrons in high magnetic fields, at commensurate filling factors[5, 6].

Second-quantization provides a general way of approaching many body systems in which the wavefunction plays a minor role. As we mentioned in chapter 3, the essence of second-quantization is a process of raising the Schrödinger wavefunction to the level of an operator which satisfies certain "canonical commutation" or "canonical anticommutation" algebras". In first quantized physics physical properties of a quantum particle, such as its density, Kinetic energy, potential energy can be expressed in terms of the one-particle wavefunction. Second quantization elevates each of these

quantities to the status of an operator by replacing the one-particle wavefuncion by its corresponding field operator:

$$\left.\begin{array}{ccc} \psi(x,t) & \rightarrow & \hat{\psi}(x,t) \\ \text{one particle wavefunction} & & \text{Field operator} \\ O(\psi^*, \psi) & \rightarrow & \hat{O}(\hat{\psi}^\dagger, \hat{\psi}) \end{array}\right\} \text{2nd Quantization} \tag{4.2}$$

For example, Born's famous expression for the one-particle (probability) density becems an operator as follows:

$$\rho(x) = |\psi(x)|^2 \rightarrow \hat{\rho}(x) = \hat{\psi}^\dagger(x)\hat{\psi}(x), \tag{4.3}$$

so that the potential energy associated with an external potential is

$$\hat{V} = \int d^3x U(x)\hat{\rho}(x). \tag{4.4}$$

Similarly, the Kinetic energy in first-quantization

$$T[\psi^*,\ \psi] = \int d^3x \psi^*(x)\left[-\frac{\hbar^2}{2m}\nabla^2\right]\psi(x) \tag{4.5}$$

becomes the operator

$$\hat{T} = \int d^3x \hat{\psi}^\dagger(x)\left[-\frac{\hbar^2}{2m}\nabla^2\right]\hat{\psi}(x). \tag{4.6}$$

Finally

$$H = \int d^3x \hat{\psi}^\dagger(x)\left[-\frac{\hbar^2}{2m}\nabla^2 + U(x)\right]\psi(x) + \frac{1}{2}\int d^3x d^3x' V(x-x') :\hat{\rho}(x)\hat{\rho}(x'): \tag{4.7}$$

is the complete many-body Hamiltonian in second-quantized form. Here $V(x-x')$ is the interaction potential between the particles, and the symbol ":" reflects the fact that order of the operators counts. ": ...:" is the normal ordering operator denotes that all creation operators between the two colons must be ordered to lie to the left of all destruction operators.

4.1 Commutation and Anticommutation Algebras

In 1928, Jordan and Wigner[7] proposed that the microscopic field operators describing identical particles divide up into two types. These are axioms of quantum field theory. For identical bosons, field operators satisfy a commutation algebra, whereas for Fermions, the field operators satisfy an *anticommutation* algebra. Since we will be dealing with many of their properties in parallel, it useful to introduce a unified notation for commutators and anticommutators as follows

$$\begin{aligned} \{a,b\} &= ab + ba \equiv [a,b]_+ , \\ [a,b] &= ab - ba \equiv [a,b]_- , \end{aligned} \tag{4.8}$$

so that

$$[a,b]_{\pm} = ab \pm ba. \tag{4.9}$$

We shall adopt the $+/-$ subscript notation in this chapter, while we are discussing both fermions and bosons together.

The algebra of field operators is then

$$\left.\begin{aligned}[\psi(1),\psi(2)]_{\pm} = [\psi^{\dagger}(2),\psi^{\dagger}(1)]_{\pm} &= 0\\ [\psi(1),\psi^{\dagger}(2)]_{\pm} &= \delta(1-2)\end{aligned}\right\}\ \textbf{Fermions/ Bosons} \tag{4.10}$$

When spin is involved, $1 \equiv (x_1,\sigma_1)$ and $\delta(1-2) = \delta^{(D)}(x_1-x_2)\delta_{\sigma_1\sigma_2}$. We shall motivate these axioms in two ways: (i) by showing, in the case of Bosons, that they are a natural result of trying to quantize the one-particle wavefunction. ; (ii) by showing that they lead to the first quantized formulation of many-body physics, naturally building the particle exchange statistics into the mathematical framework.

Table 5.1 summarizes the main points of second-quantization that we shall now discuss in detail.

4.1.1 Heuristic Derivation for Bosons

The name second-quantization derives from the notion that many body physics can be obtained by quantizing the one-particle wavefunction. Philosophically, this is very tricky, for surely, the wavefunction is already a quantum object? Let us imagine however, a thought experiment, when we prepare a huge number of non-interacting particles, prepared in such a way that they are all in precisely the same quantum state. The feasibility of this does not worry us here, but note that it can actually be done for a large ensemble of bosons, by condensing them into a single quantum state. In this circumstance, every single particle lies in the same one-particle state. If we time evolve the system we can begin to think of the single-particle wavefunction as if it is a classical variable.

Let us briefly recall one-particle quantum mechanics. If the particle is in a state $|\psi\rangle$, then we can always expand the state in terms of a complete basis $\{|n\rangle\}$, as follows:

$$|\psi(t)\rangle = \sum_n |n\rangle \overbrace{\langle n|\psi(t)\rangle}^{\psi_n(t)} = \sum_n |n\rangle\psi_n(t) \tag{4.11}$$

so that $|\psi_n(t)|^2 = p_n(t)$ gives the probability of being in state n. Now applying Schrodinger's equation, $\hat{H}|\psi\rangle = i\hbar\partial_t|\psi\rangle$ gives

$$\begin{aligned} i\hbar\dot{\psi}_n(t) &= \sum_m \langle n|H|m\rangle\psi_m(t)\\ i\hbar\dot{\psi}^*_n(t) &= -\sum_m \langle m|H|n\rangle\psi^*_m(t)\end{aligned} \tag{4.12}$$

Now if we write the ground-state energy as a functional of the $b_m(t)$, we get

$$H(\psi,\psi^*) = \langle H\rangle = \sum_{m,n}\psi^*_m\psi_n\langle m|H|n\rangle \tag{4.13}$$

Table. 5.1. First and Second Quantization treatment of conserved particles.

	First Quantization	Second Quantization
Wavefn $\longrightarrow$ Field Operator	$\psi(x) = \langle x\|\psi\rangle$	$\hat{\psi}(x)$
Commutator	$[x,p] = i\hbar$	$[\hat{\psi}(x),\hat{\psi}^{\dagger}(x')]_{\mp} = \delta^D(x-x')$
Density	$\rho(x) = \|\psi(x)\|^2$	$\hat{\rho}(x) = \hat{\psi}^{\dagger}(x)\hat{\psi}(x)$
Arbitrary Basis	$\psi_{\lambda} = \langle\lambda\|\psi\rangle$	$\hat{\psi}_{\lambda}$
Change of Basis	$\langle\vec{s}\|\psi\rangle = \sum_{\lambda}\langle\vec{s}\|\lambda\rangle\langle\lambda\|\psi\rangle$	$\hat{a}_s = \sum_{\lambda}\langle\vec{s}\|\lambda\rangle\hat{\psi}_{\lambda}$
Orthogonality	$\langle\lambda\|\lambda'\rangle = \delta_{\lambda\lambda'}$	$[\psi_{\lambda},\psi^{\dagger}{}_{\lambda'}]_{\mp} = \delta_{\lambda\lambda'}$
One ptcle Energy	$\frac{p^2}{2m} + U$	$\int_x \hat{\psi}^{\dagger}(x)\Big(-\frac{\hbar^2}{2m} + U(x)\Big)\hat{\psi}(x)$
Interaction	$\sum_{i<j} V(x_i - x_j)$	$\hat{V} = \frac{1}{2}\int_{x,x'} V(x-x') : \hat{\rho}(x)\hat{\rho}(x') :$ $= \frac{1}{2}\sum V(\mathbf{q})c^{\dagger}{}_{\mathbf{k}+\mathbf{q}}c^{\dagger}{}_{\mathbf{k}'-\mathbf{q}}c_{\mathbf{k}'}c_{\mathbf{k}}$
Many Body Wavefunction	$\Psi(x_1,x_2\ldots x_N)$	$\langle 0\|\hat{\psi}(x_1)\ldots\hat{\psi}(x_N)\|0\rangle$
Schrödinger Eqn	$\Big(\sum \mathcal{H}_i + \sum_{i<j} V_{ij}\Big)\Psi = i\hbar\dot{\Psi}$	$[\mathcal{H}^{(0)} + \int_{x'}\hat{\rho}(x')V(x'-x)]\hat{\psi}(x) = i\hbar\dot{\psi}(x)$

we see that the equations of motion can be written in Hamiltonian form

$$\begin{aligned} \dot{\psi}_m &= \frac{\partial H(\psi,\psi^*)}{i\hbar\partial\psi^*_m}, \qquad (\text{c.f } \dot{q} = \frac{\partial H}{\partial p})\\ i\hbar\dot{\psi}^*_m &= -\frac{\partial H(\psi,\psi^*)}{\partial\psi_m}, \qquad (\text{c.f } \dot{p} = -\frac{\partial H}{\partial q})\end{aligned} \tag{4.14}$$

so we can identify

$$\{\psi_n, i\hbar\psi^*_n\} \equiv \{q_n, p_n\} \tag{4.15}$$

as the canonical position and momentum co-ordinates.

But suppose we don't have a macroscopic number of particles in a single state. In this case, the amplitudes $\psi_n(t)$ are expected to undergo quantum fluctuations. Let us examine what happens if we "second-quantize" these variables, making the replacement

$$[q_n,\ p_m] = i\hbar\delta_{nm} = i\hbar[\psi_n,\psi^{\dagger}{}_m] \tag{4.16}$$

or

$$\boxed{\begin{aligned}[\psi_n, \psi_m] &= [\psi^\dagger{}_n, \psi^\dagger{}_m] = 0, \\ [\psi_n, \psi^\dagger{}_m] &= \delta_{nm}\end{aligned}} \tag{4.17}$$

In terms of these operators, our second quantized Hamiltonian becomes

$$H = \sum_{m,l} \hat{\psi}^\dagger{}_m \hat{\psi}_l \langle m|H|l\rangle \tag{4.18}$$

If we now use this to calculate the time-evolution of the quantum fields we obtain

$$-i\hbar\partial_t \psi_j = [\hat{H},\ \psi_j] = \sum_{m,l} \langle m|H|l\rangle \overbrace{[\psi^\dagger{}_m \psi_l, \psi_j]}^{-\delta_{mj}\psi_l} \tag{4.19}$$

Eliminating the sum over m, we obtain

$$\begin{aligned} -i\hbar\partial_t \psi_j &= -\sum_l \langle j|H|l\rangle \psi_l \\ -i\hbar\partial_t \psi^\dagger{}_j &= [\hat{H},\ \psi^\dagger{}_j] = \sum_l \psi^\dagger{}_l \langle l|H|j\rangle, \end{aligned} \tag{4.20}$$

where the complex conjugated expression gives the time evolution of $\psi^\dagger{}_l$. Remarkably, the equations of motion of the operators match the time evolution of the one-particle amplitudes. But now we have operators, we have all the new physics associated with quantum fluctuations of the particle fields.

4.2 What about Fermions?

Remarkably, as Jordan and Wigner first realized, we recover precisely the same time-evolution if second-quantize the operators using anticommutators[7], rather than commutators, and it this is what gives rise to fermions and the exclusion principle. But for fermions, we can not offer a heurtistic argument, because they don't condense: as far as we know, there is no situation in which individual fermi field operators behave semi-classically. although of course, in a superconductor, pairs of fermions that behave semi-classically.

In fact, all of the operations we carried out above work equally well with either canonical commutation or canonical *anticomutation* relations:

$$\boxed{\begin{aligned}[\psi_n, \psi_m]_\pm &= [\psi^\dagger{}_n, \psi^\dagger{}_m]_\pm = 0, \\ [\psi_n, \psi^\dagger{}_m]_\pm &= \delta_{nm}\end{aligned}} \tag{4.21}$$

where the ± refers to fermions/bosons respectively.

To evaluate the equation of motion of the field operators, we need to know the commutator $[H, \psi_n]$. Using the relation

$$[ab, c] = a[b, c]_\pm \mp [a, c]_\pm b \tag{4.22}$$

we may verify that

$$\begin{aligned} [\psi^\dagger{}_m \psi_l, \psi_j] &= \psi^\dagger{}_m \overbrace{[\psi_l, \psi_j]}^{0}{}_\pm \mp \overbrace{[\psi^\dagger{}_m, \psi_j]_\pm}^{-\delta_{mj}} \psi_l \\ &= -\delta_{mj}\psi_l \end{aligned} \tag{4.23}$$

so that

$$\begin{aligned} -i\hbar\partial_t \psi_j &= [\hat{H},\ \psi_j] = \sum_{m,l} \langle m|H|l\rangle \overbrace{[\psi^\dagger{}_m \psi_l, \psi_j]}^{-\delta_{mj}\psi_l} \\ &= -\sum_l \langle j|H|l\rangle \psi_l \end{aligned} \tag{4.24}$$

independently of whether we use an anticommuting, or commuting algebra.

Let us now go on, and look at some general properties of second-quantized operators that hold for both bosons and fermions.

4.3 Field operators in different bases

Let us first check that our results don't depend on the one-particle basis we use. To do this, we must confirm that the commutation or anticommutation algebra of bosons or fermions is basis independent. Suppose we have two bases of one-particle states: the $\{|r\rangle\}$ basis, and a new $\{|\bar{s}\rangle\}$ basis, where

$$|\psi\rangle = \sum_r |r\rangle \psi_r = \sum_s |\bar{s}\rangle a_s \tag{4.25}$$

where $\langle \bar{s}|\psi\rangle = a_s$, $\langle r|\psi\rangle = \psi_r$. Introducing the completeness relation $1 = \sum_r |r\rangle\langle r|$ into the first expression, we obtain

$$\overbrace{\langle \bar{s}|\psi\rangle}^{a_s} = \sum_r \langle \bar{s}|r\rangle \overbrace{\langle r|\psi\rangle}^{\psi_s} \tag{4.26}$$

If this is how the one-particle states transform between the two bases, then we must use the same unitary transformation to relate the field operators that destroy particles in the two bases

$$\hat{a}_s = \sum_r \langle \bar{s}|r\rangle \hat{\psi}_r \tag{4.27}$$

The commutation algebra of the new operators is now

$$[\hat{a}_s, \hat{a}^\dagger{}_p]_\pm = \sum_{l,m} \langle \bar{s}|l\rangle \overbrace{[\hat{\psi}_l, \hat{\psi}^\dagger{}_m]_\pm}^{\delta_{lm}} \langle m|\bar{p}\rangle \tag{4.28}$$

This is just the pre- and post-multiplication of a unit operator by the unitary matrix $U_{sl} = \langle \bar{s}|l\rangle$ and its conjugate $U^\dagger_{mp} = \langle m|\bar{p}\rangle$. The final result, is unity, as expected:

$$[\hat{a}_s, \hat{a}^\dagger{}_p]_\pm = \sum_r \langle \bar{s}|r\rangle\langle r|\bar{p}\rangle = \langle \bar{s}|\bar{p}\rangle = \delta_{sp} \tag{4.29}$$

In other words, the canonical commutation algebra is preserved by unitary transformations of basis.

A basis of particular importance, is the position basis. The one-particle wavefunction can always be decomposed in a discrete basis, as follows

$$\psi(x) = \langle x|\psi(t)\rangle = \sum_n \langle x|n\rangle\psi_n \tag{4.30}$$

where $\langle x|n\rangle = \phi_n(x)$ is the wavefunction of the nth state. We now define the corresponding destruction operator

$$\hat{\psi}(x) = \sum_m \langle x|m\rangle\hat{\psi}_m \tag{4.31}$$

which defines the field operator in real space. Using completeness of the one-particle eigenstates $1 = \int d^D x|x\rangle\langle x|$, we can expand the orthogonality relation $\delta_{nm} = \langle n|m\rangle$ as

$$\delta_{nm} = \langle n| \overbrace{\hat{1}}^{1=\int d^D x|x\rangle\langle x|} |m\rangle = \int d^D x \langle n|x\rangle\langle x|m\rangle.$$

By integrating (4.31) over x with $\langle n|x\rangle$, we can then invert this equation to obtain

$$\psi_n = \int d^D x \langle n|x\rangle\psi(x), \qquad \psi^\dagger{}_n = \int d^D x \psi^\dagger(x)\langle x|n\rangle \tag{4.32}$$

You can see by now, that so far as transformation laws are concerned, $\psi_n \sim \langle n|$ and $\psi(x) \sim \langle x|$ transforms like "bra" vectors, whilst their conjugates transform like "kets".

By moving to a real-space representation, we have traded in a discrete basis, for a continuous basis. The corresponding "unit" operator appearing in the commutation algebra now becomes a delta-function.

$$\begin{aligned}[\psi(x), \psi^\dagger(y)]_\pm &= \sum_{n,m} \langle x|n\rangle\langle m|y\rangle \overbrace{[\psi_n,\ \psi^\dagger{}_m]_\pm}^{\delta_{nm}} \\ &= \sum_n \langle x|n\rangle\langle n|y\rangle = \langle x|y\rangle \\ &= \delta^3(x-y)\end{aligned} \tag{4.33}$$

where we have assumed a three-dimensional system.

Another basis of importance, is the basis provided by the one-particle energy eigenstates. In this basis $\langle l|H|m\rangle = E_l\delta_{lm}$, so the Hamiltonian becomes diagonal

$$H = \sum_l E_l \psi^\dagger{}_l\psi_l = \sum E_l \hat{n}_l \tag{4.34}$$

The Hamiltonian of the non-interacting many-body system thus divides up into a set of individual components, each one describing the energy associated with the occupancy of a given one-particle eigenstate. The eigenstates of the many-body Hamiltonian are thus labelled by the occupancy of the lth one-particle state. Of course, in a real-space basis the Hamiltonian becomes more complicated. Formally, if we transform this back to the real-space basis, we find that

$$H = \int d^D x d^D x' \psi^\dagger(x)\langle x|H|x'\rangle\psi(x') \tag{4.35}$$

For free particles in space, the one-particle Hamiltonian is

$$\langle x|H|x'\rangle = \Big[-\frac{\hbar^2}{2m}\nabla^2 + U(x)\Big]\delta^D(x-x') \tag{4.36}$$

so that the Hamiltonian becomes

$$H = \int d^D x \psi^\dagger(x)\Big[-\frac{\hbar^2}{2m}\nabla^2 + U(x)\Big]\psi(x) \tag{4.37}$$

which despite its formidable appearance, is just a a transformed version of the diagonalized Hamiltonian (4.34).

Example 4.1: By integrating by parts, taking care with the treatment of surface terms, show that the second quantized expression Hamiltonian (4.37) can be re-written in the form

$$H = \int d^D x \left(\frac{\hbar^2}{2m}|\nabla\psi(x)|^2 + U(x)|\psi(x)|^2\right), \tag{4.38}$$

where we have taken a notational liberty common in field theory, denoting $|\nabla\psi(x)|^2 \equiv \vec{\nabla}\psi^\dagger(x)\cdot\vec{\nabla}\psi(x)$ and $|\psi(x)|^2 \equiv \psi^\dagger(x)\psi(x)$.

Solution: Let us concentrate on the kinetic energy term in the Hamiltonian, writing $H = T + U$, where

$$T = \int d^D x \psi^\dagger(x)\left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi(x). \tag{4.39}$$

Integrating this term by parts we can split it into a "bulk" and a "surface" term, as follows:

$$T = -\frac{\hbar^2}{2m}\int d^D x \vec{\nabla}\psi^\dagger(x)\cdot\vec{\nabla}\psi(x) + \frac{\hbar^2}{2m}\overbrace{\int d^D x \vec{\nabla}\cdot\left(\psi^\dagger(x)\vec{\nabla}\psi(x)\right)}^{T_S}. \tag{4.40}$$

Using the divergence theorem, we can rewrite the total derivative as a surface integral

$$T_S = -\frac{\hbar^2}{2m}\int d\vec{S}\cdot\left(\psi^\dagger(x)\vec{\nabla}\psi(x)\right) \tag{4.41}$$

Now it is tempting to just drop this term as a surface term that "vanishes at infinity". However, here we are dealing with operators, so this brash step requires a little contemplation before we

take it for granted. One way to deal with this term is to use periodic boundary conditions. In this case there really are no boundaries, or more strictly speaking, opposite boundaries cancel ($\int_R dS + \int_L dS = 0$), so the surface term is zero. But suppose we had used hard wall boundary conditions, what then?

Well, in this case, we can decompose the field operators in terms of the one-particle eigenstates of the cavity. Remembering that under change of bases, $\psi(x) \sim \langle x|$ and $\psi^\dagger(x) \sim |x\rangle$ behave as bras and kets respectively, we write

$$\psi(x) = \sum_n \overbrace{\langle x|n\rangle}^{\phi_n(x)} \psi_n, \qquad \psi^\dagger(x) = \sum_n \psi^\dagger{}_n \overbrace{\langle n|x\rangle}^{\phi_n^*(x)}.$$

Substituting these expressions into T_S (4.41), the surface term becomes

$$\begin{aligned} T_S &= \sum_{n,m} t^{(S)}_{nm} \psi^\dagger{}_n \psi_m \\ t^S_{nm} &= -\frac{\hbar^2}{2m} \int d\vec{S} \cdot \phi_n^*(x) \vec{\nabla} \phi_m(x) \end{aligned} \tag{4.42}$$

Provided $\phi_n(x) = 0$ on the surface, it follows that the matrix elements $t^S_{nm} = 0$ so that $\hat{T}_S = 0$.

Thus whether we use hard-wall or periodic boundary conditions, we can drop the surface contribution to the Kinetic energy in (4.40), enabling us to write

$$T = \frac{\hbar^2}{2m} \int d^D x |\vec{\nabla}\psi(x)|^2$$

and when we add in the potential term, we obtain (4.38).

4.4 Fields as particle creation and annihilation operators.

By analogy with collective fields, we now interpret the quantity $\hat{n}_l = \psi^\dagger{}_l \psi_l$ as the number number operator, counting the number of particles in the one-particle state l. The total particle number operator is then

$$N = \sum_l \psi^\dagger{}_l \psi_l \tag{4.43}$$

Using relation (4.22), it is easy to verify that for both fermions and bosons,

$$[\hat{N}, \psi_l] = [\hat{n}_l, \psi_l] = -\psi_l, \qquad [\hat{N}, \psi^\dagger{}_l] = [\hat{n}_l, \psi^\dagger{}_l] = \psi^\dagger{}_l. \tag{4.44}$$

In other words, $\hat{N}\psi^\dagger{}_l = \psi^\dagger{}_l(\hat{N}+1)$ so that $\psi^\dagger{}_l$ adds a particle to state l. Similarly, since $\hat{N}\psi_l = \psi_l(\hat{N}-1)$, ψ_l *destroys* a particle from state l.

There is however a vital and essential difference between bosons and fermions. For bosons, the

number of particles n_l in the *lth* state is unbounded, but for fermions, since

$$\psi^{\dagger 2}_l = \frac{1}{2}\{\psi^\dagger{}_l, \psi^\dagger{}_l\} = 0 \tag{4.45}$$

the amplitude to add more than one particle to a given state is always zero. We can never add more than one particle to a given state: in otherwords, the *exclusion principle* follows from the algebra! The occupation number bases for bosons and fermions are given by

$$\boxed{\begin{aligned} |n_1, n_2 \ldots n_l \ldots\rangle &= \prod_l \tfrac{(\psi^\dagger_l)^{n_l}}{\sqrt{n_l!}}|0\rangle, \qquad (n_r = 0, 1, 2 \ldots) \quad \textbf{bosons} \\ |n_1, n_2 \ldots n_r\rangle &= (\psi^\dagger{}_r)^{n_r} \ldots (\psi^\dagger{}_1)^{n_1}|0\rangle, \quad (n_r = 0, 1) \qquad \textbf{fermions} \end{aligned}} \tag{4.46}$$

A specific example for fermions, is

$$|\overset{1\,2\,3\,4\,5\,6}{1\,0\,1\,1\,0\,1}\rangle = \psi^\dagger{}_6 \psi^\dagger{}_4 \psi^\dagger{}_3 \psi^\dagger{}_1 |0\rangle \tag{4.47}$$

which contains particles in the 1st, 3rd, 4th and 6th one-particle states. Notice how the *order* in which we add the particles affects the sign of the wavefunction, so exchanging particles 4 and 6 gives

$$\psi^\dagger{}_4 \psi^\dagger{}_6 \psi^\dagger{}_3 \psi^\dagger{}_1 |0\rangle = -\psi^\dagger{}_6 \psi^\dagger{}_4 \psi^\dagger{}_3 \psi^\dagger{}_1 |0\rangle = -|\overset{1\,2\,3\,4\,5\,6}{1\,0\,1\,1\,0\,1}\rangle \tag{4.48}$$

By contrast, a bosonic state is symmetric, for example

$$|\overset{1\,2\,3\,4\,5\,6}{8\,0\,5\,2\,4\,1}\rangle = \frac{1}{\sqrt{4!2!5!8!}} \psi^\dagger{}_6 (\psi^\dagger{}_5)^4 (\psi^\dagger{}_4)^2 (\psi^\dagger{}_3)^5 (\psi^\dagger{}_1)^8 |0\rangle \tag{4.49}$$

To get further insight, let us transform the number operator to a real-space basis by writing

$$\hat{N} = \int d^D x d^D y \sum_l \psi^\dagger(x) \overbrace{\langle x|l\rangle\langle l|y\rangle}^{\delta^D(x-y)} \psi(y) \tag{4.50}$$

so that

$$\hat{N} = \int d^D x \psi^\dagger(x)\psi(x) \tag{4.51}$$

From this expression, we are immediately led to identify

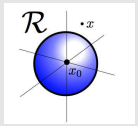
$$\rho(x) = \psi^\dagger(x)\psi(x) \tag{4.52}$$

as the density operator. Furthermore, since

$$[\rho(y), \psi(x)] = \mp[\psi^\dagger(y), \psi(x)] \pm \psi(y) = -\delta^3(x-y)\psi(y). \tag{4.53}$$

we can we can identify $\psi(x)$ as the operator which annihilates a particle at x.

Example 4.2: Using the result (4.53) that if



$$\hat{N}_{\mathcal{R}} = \int_{y\in\mathcal{R}} d^3y\rho(\vec{y}) \tag{4.54}$$

measures the number of particles in some region $\mathcal{R}$, that

$$[\hat{N}_{\mathcal{R}}, \psi(x)] = \begin{cases} -\psi(x), & (x \in \mathcal{R}) \\ 0 & (x \notin \mathcal{R}) \end{cases} \tag{4.55}$$

By localizing region $\mathcal{R}$ around x_0, use this to prove that $\psi(x_0)$ annihilates a particle at position x_0.

Solution: By directly commuting $\hat{N}_{\mathcal{R}}$ with $\psi(x)$, we obtain

$$[\hat{N}_{\mathcal{R}}, \psi(x)] = \int_{y\in\mathcal{R}} [\rho(y), \psi(x)] = -\int_{y\in\mathcal{R}} \delta^3(x-y)\psi(y) = \begin{cases} -\psi(x), & (x \in \mathcal{R}) \\ 0 & (x \notin \mathcal{R}) \end{cases}$$

Suppose $|n_{\mathcal{R}}\rangle$ is a state with a definite number $n_{\mathcal{R}}$ of particles inside $\mathcal{R}$. If the region $\mathcal{R}$ is centered around x_0, then it follows that

$$\hat{N}_{\mathcal{R}}\psi(x_0)|n_{\mathcal{R}}\rangle = \psi(x_0)(\hat{N}_{\mathcal{R}} - 1)|n_{\mathcal{R}}\rangle = (n_{\mathcal{R}} - 1)\psi(x_0)|n_{\mathcal{R}}\rangle$$

contains one less particle. In this way, we see that $\psi(x)$ annihilates a particle from inside region $\mathcal{R}$, no matter how small that region is made, proving that $\psi(x)$ annihilates a particle at position x_0.

Example 4.3: Suppose $b_{\vec{q}}$ destroys a boson in a cubic box of side length L,where $\vec{q} = \frac{2\pi}{L}(i, j, k)$ is the momentum of the boson. Express the field operators in real space, and show they satisfy canonical commutation relations. Write down the Hamiltonian in both bases.

Solution The field operators in momentum space satisfy $[b_{\vec{q}}, b^\dagger_{\vec{q}'}] = \delta_{\vec{q}\vec{q}'}$. We may expand the field operator in real space as follows

$$\psi(x) = \sum_{\mathbf{q}} \langle\vec{x}|\vec{q}\rangle b_{\vec{q}} \tag{4.56}$$

Now

$$\langle\vec{x}|\vec{q}\rangle = \frac{1}{L^{3/2}} e^{i\vec{q}\cdot\vec{x}} \tag{4.57}$$

is the one-particle wavefunction of a boson with momentum $\vec{q}$. Calculating the commutator between the fields in real space, we obtain

$$[\psi(\vec{x}), \psi^\dagger(\vec{y})] = \sum_{\vec{q},\vec{q}'} \langle\vec{x}|\vec{q}\rangle\langle\vec{q}'|\vec{y}\rangle \overbrace{[b_{\vec{q}}, b^\dagger_{\vec{q}'}]}^{\delta_{\vec{q}\vec{q}'}} = \sum_{\vec{q}} \langle\vec{x}|\vec{q}\rangle\langle\vec{q}|\vec{y}\rangle$$

$$= \frac{1}{L^3}\sum_{\mathbf{q}} e^{i\vec{q}\cdot(\vec{x}-\vec{y})} = \delta^{(3)}(\vec{x}-\vec{y}). \tag{4.58}$$

The last two steps could have been carried out by noting that $\sum_q |q\rangle\langle q| = 1$, so that $[\psi(\vec{x}), \psi^\dagger(\vec{y})] = \langle x|y\rangle = \delta^3(x-y)$.

The Hamiltonian for the bosons in a box is

$$H = -\frac{\hbar^2}{2m}\int d^3x\psi^\dagger(x)\nabla^2\psi(x) \tag{4.59}$$

We now Fourier transform this, writing

$$\begin{aligned} \psi^\dagger(x) &= \frac{1}{L^{3/2}}\sum_{\mathbf{q}} e^{-i\vec{q}\cdot\vec{x}} b^\dagger{}_{\mathbf{q}} \\ \nabla^2\psi(x) &= -\frac{1}{L^{3/2}}\sum_{\mathbf{q}} q^2 e^{i\vec{q}\cdot\vec{x}} b_{\mathbf{q}} \end{aligned} \tag{4.60}$$

Substituting into the Hamiltonian, we obtain

$$H = \frac{1}{L^3}\sum_{\mathbf{q},\,\mathbf{q}'} \epsilon_{\mathbf{q}} b^\dagger{}_{\mathbf{q}'} b_{\mathbf{q}} \int d^3x \overbrace{e^{i\mathbf{q}-\mathbf{q}'\cdot\mathbf{x}}}^{L^3\delta_{\vec{q}-\vec{q}'}} = \sum_{\mathbf{q}} \epsilon_{\mathbf{q}} b^\dagger{}_{\mathbf{q}} b_{\mathbf{q}}, \tag{4.61}$$

where

$$\epsilon_{\mathbf{q}} = \left(\frac{\hbar^2 q^2}{2m}\right). \tag{4.62}$$

is the one-particle energy.

4.5 The vacuum and the many body wavefunction

We are now in a position to build up the many-body wavefunction. Once again, of fundamental importance here, is the notion of the vacuum, the unique state $|0\rangle$ which is annihilated by all field operators. If we work in the position basis, we can add a particle at site x to make the one-particle state

$$|x\rangle = \psi^\dagger(x)|0\rangle, \tag{4.63}$$

Notice that the overlap between two one-particle states is

$$\langle x|x'\rangle = \langle 0|\psi(x)\psi^\dagger(x')|0\rangle. \tag{4.64}$$

By using the (anti) commutation algebra to move the creation operator in the above expression to the right-hand side, where it annihilates the vacuum, we obtain

$$\langle 0|\psi(x)\psi^\dagger(x')|0\rangle = \langle 0|\overbrace{[\psi(x),\ \psi^\dagger(x')]_\pm}^{\delta^{(3)}(x-x')}|0\rangle = \delta^{(3)}(x-x'). \tag{4.65}$$

We can equally well add many particles, forming the N-particle state:

$$|x_1, x_2 \ldots x_N\rangle = \psi^\dagger(x_N)\ldots\psi^\dagger(x_2)\psi^\dagger(x_1)|0\rangle \tag{4.66}$$

Now the corresponding "bra" state is given by

$$\langle x_1, x_2 \ldots x_N| = \langle 0|\psi(x_1)\psi(x_2)\ldots\psi(x_N) \tag{4.67}$$

The wavefunction of the N-particle state Ψ is the overlap with this state

$$\boxed{\Psi(x_1, x_2, \ldots x_N) = \langle x_1, x_2 \ldots x_N|\Psi\rangle = \langle 0|\psi(x_1)\psi(x_2)\ldots\psi(x_N)|\Psi\rangle} \tag{4.68}$$

The commutation/anticommutation algebra guarantees that the symmetry of this wavefunction under particle exchange is positive for bosons, and negative for fermions, so that if we permute the particles, $(12\ldots N) \to (P_1 P_2 \ldots P_N)$

$$\langle 0|\psi(x_{P_1})\psi(x_{P_2})\ldots\psi(x_{P_N})|\Psi\rangle = (\mp 1)^P\langle 0|\psi^\dagger(x_1)\psi(x_2)\ldots\psi(x_N)|\Psi\rangle \tag{4.69}$$

where P is the number of pairwise permutations involved in making the permutation. Notice that for fermions, this hard-wires the Pauli Exclusion principle into the formalism, and guarantees a node in the wavefunction when any two particle co-ordinates are the same.

Example Two spinless fermions are added to a cubic box with sides of length L, in momentum states k_1 and k_2, forming the state

$$|\Psi\rangle = |\mathbf{k}_1, \mathbf{k}_2\rangle = c^\dagger_{\mathbf{k}_2} c^\dagger_{\mathbf{k}_1}|0\rangle \tag{4.70}$$

Calculate the two-particle wavefunction

$$\Psi(x_1, x_2) = \langle x_1, x_2|\Psi\rangle \tag{4.71}$$

Solution Written out explicitly, the wavefunction is

$$\Psi(x_1, x_2) = \langle 0|\psi(x_1)\psi(x_2)c^\dagger_{\mathbf{k}_2} c^\dagger_{\mathbf{k}_1}|0\rangle \tag{4.72}$$

To evaluate this quantity, we commute the two destruction operators to the right, until they annihilate the vacuum. Each time a destruction operator passes a creation operator, we generate a "contraction" term

$$\{\psi(x), c^\dagger_{\mathbf{k}}\} = \int d^3y \overbrace{\{\psi(x), \psi^\dagger(y)\}}^{\delta^3(x-y)}\langle y|\mathbf{k}\rangle = \langle x|\mathbf{k}\rangle = L^{-3/2}e^{i\mathbf{k}\cdot\mathbf{x}} \tag{4.73}$$

Carrying out this procedure, we generate a sum of pairwise contractions, as follows:

$$\begin{aligned}\langle 0|\psi(x_1)\psi(x_2)c^\dagger_{\mathbf{k}_2} c^\dagger_{\mathbf{k}_1}|0\rangle &= \langle x_1|\mathbf{k}_1\rangle\langle x_2|\mathbf{k}_2\rangle - \langle x_1|\mathbf{k}_2\rangle\langle x_2|\mathbf{k}_1\rangle \\ &= \frac{1}{L^3}\Big[e^{i(\mathbf{k}_1\cdot\mathbf{x}_1 + \mathbf{k}_2\cdot\mathbf{x}_2)} - e^{i(\mathbf{k}_1\cdot\mathbf{x}_2 + \mathbf{k}_2\cdot\mathbf{x}_1)}\Big]\end{aligned}$$

4.6 Interactions

Second-quantization is easily extended to incorporate interactions. Classically, the interaction potential energy between particles is given by

$$V = \frac{1}{2}\int d^3x d^3x' V(x - x')\rho(x)\rho(x') \tag{4.74}$$

so we might expect that the corresponding second-quantized expression is

$$\frac{1}{2}\int d^3x d^3x' V(x - x')\hat{\rho}(x)\hat{\rho}(x') \tag{4.75}$$

This is wrong, because we have not been careful about the ordering of operators. Were we to use (4.75), then a one-particle state would interact with itself! We require that the action of the potential on the vacuum, or a one-particle state, gives zero

$$\hat{V}|0\rangle = \hat{V}|x\rangle = 0 \tag{4.76}$$

To guarantee this, we need to be careful that we "normal-order" the field operators, by permuting them so that all destruction operators are on the right-hand-side. All additional terms that are generated by permuting the operators are dropperd, but the signs associated with the permutation process are preserved. We denote the normal ordering process by two semi-colons. Thus

$$\begin{aligned}:\rho(x)\rho(y): &= :\psi^\dagger(x)\psi(x)\psi^\dagger(y)\psi(y): \\ &= \mp :\psi^\dagger(x)\psi^\dagger(y)\psi(x)\psi(y): =: \psi^\dagger(y)\psi^\dagger(x)\psi(x)\psi(y):\end{aligned} \tag{4.77}$$

and the correct expression for the interaction potential is then

$$\begin{aligned}V &= \frac{1}{2}\int d^3x d^3x' V(x - x') :\hat{\rho}(x)\hat{\rho}(x'): \\ &= \sum_{\sigma,\sigma'}\frac{1}{2}\int d^3x d^3x' V(x - x')\psi_\sigma{}^\dagger(y)\psi_{\sigma'}{}^\dagger(x)\psi_{\sigma'}(x)\psi_\sigma(y)\end{aligned} \tag{4.78}$$

where we have written a more general expression for fields with spin.

Example. Show that the action of the operator V on the many body state $|x_1, \ldots x_N\rangle$ is given by

$$\hat{V}|x_1, x_2, \ldots x_N\rangle = \sum_{i<j} V(x_i - x_j)|x_1, x_2, \ldots x_N\rangle \tag{4.79}$$

Solution: To prove this, we first prove the intermediate result

$$[\hat{V}, \psi^\dagger(x)] = \int d^3y V(x - y)\psi^\dagger(x)\rho(y). \tag{4.80}$$

This result can be obtained by expanding out the commutator as follows:

$$\begin{aligned}[\hat{V},\psi^\dagger(x)] &= \frac{1}{2}\int_{y,y'} V(y-y')\psi^\dagger(y)\psi^\dagger(y')\overbrace{[\psi(y')\psi(y),\psi^\dagger(x)]}^{\delta(y-x)\psi(y')\pm\delta(y'-x)\psi(y)} \\ &= \psi^\dagger(x)\frac{1}{2}\int_{y'} V(x-y')\rho(y') \pm \frac{1}{2}\int_y V(y-x)\overbrace{\psi^\dagger(y)\psi^\dagger(x)}^{\pm\psi^\dagger(x)\psi^\dagger(y)}\psi(y) \\ &= \int_y V(x-y)\psi^\dagger(x)\rho(y), \end{aligned} \tag{4.81}$$

where the lower sign choice is for fermions.

We now calculate

$$\hat{V}|x_1,\ldots x_N\rangle = \hat{V}\psi^\dagger(x_N)\ldots\psi^\dagger(x_1)|0\rangle \tag{4.82}$$

by commuting $\hat{V}$ successively to the right until it annihilates with the vacuum. At each stage, we generate a "remainder term". When we commute it past the the "jth" creation operator we obtain

$$\psi^\dagger(x_N)\ldots\hat{V}\psi^\dagger(x_j)\ldots\psi^\dagger(x_1)|0\rangle = \psi^\dagger(x_N)\ldots\psi^\dagger(x_j)\hat{V}\ldots\psi^\dagger(x_1)|0\rangle + \mathcal{R}_j \tag{4.83}$$

where the remainder is

$$\mathcal{R}_j = \int d^3y\psi^\dagger(x_N)\ldots V(y-x_j)\psi^\dagger(x_j)\rho(y)\ldots\psi^\dagger(x_1)|0\rangle \tag{4.84}$$

Next, using $\rho(y)\psi^\dagger(x_i) = \psi^\dagger(x_i)\rho(y) + \psi^\dagger(x_i)\delta(y-x_i)$, we commute the density operator to the right until it annihilates the vacuum. The remainder terms generated by this process are then

$$\begin{aligned}\mathcal{R}_j &= \sum_{i=1}^{j-1} V(x_i-x_j)\psi^\dagger(x_N)\ldots\psi^\dagger(x_j)\ldots\psi^\dagger(x_i)\ldots\psi^\dagger(x_1)|0\rangle \\ &= \sum_{i=1}^{j-1} V(x_i-x_j)|x_1,x_2\ldots x_N\rangle. \end{aligned} \tag{4.85}$$

Our final answer is the sum of the remainders $\mathcal{R}_j$:

$$\begin{aligned}\hat{V}\psi^\dagger(x_N)\ldots\psi^\dagger(x_1)|0\rangle &= \sum_{j=2,N}\mathcal{R}_j \\ &= \sum_{i<j} V(x_i-x_j)|x_1,x_2\ldots x_N\rangle. \end{aligned} \tag{4.86}$$

In otherwords, the state $|x_1\ldots x_N\rangle$ is an eigenstate of the interaction operator, with eigenvalue given by the classical interaction potential energy.

To get another insight into the interaction, we shall now rewrite it in the momentum basis. This is very useful in translationally invariant systems, where momentum is conserved in collisions. Let

us imagine we are treating fermions, with spin. The transformation to a momentum basis is then Writing

$$\begin{aligned}\psi_\sigma(x) &= \text{“}\sum_{\mathbf{k}}\text{”}\langle\mathbf{x}|\mathbf{k}\rangle c_{\mathbf{k}\sigma} = \int_{\mathbf{k}} c_{\mathbf{k}\sigma}e^{i(\mathbf{k}\cdot\mathbf{x})} \\ \psi_\sigma(x) &= \text{“}\sum_{\mathbf{k}}\text{”}c^\dagger{}_{\mathbf{k}\sigma}\langle\mathbf{k}|\mathbf{x}\rangle = \int_{\mathbf{k}} c^\dagger{}_{\mathbf{k}\sigma}e^{-i(\mathbf{k}\cdot\mathbf{x})} \end{aligned} \tag{4.87}$$

where $\{c_{\mathbf{k}\sigma}, c^\dagger{}_{\mathbf{k}'\sigma'}\} = (2\pi)^3\delta^3(\mathbf{k}-\mathbf{k}')\delta_{\sigma\sigma'}$ are canonical fermion operators and we have used the short-hand notation

$$\int_{\mathbf{k}} = \int\frac{d^3k}{(2\pi)^3}. \tag{4.88}$$

We shall also Fourier transform the interaction

$$V(x-x') = \int_{\mathbf{q}} V(\mathbf{q})e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')}. \tag{4.89}$$

When we substitute these expressions into the interaction, we need to regroup the Fourier terms so that the momentum integrals are on the outside, and the spatial integrals are on the inside. Doing this, we obtain

$$\hat{V} = \frac{1}{2}\sum_{\sigma\sigma'}\int_{\mathbf{k}_{1,2,3,4}} V(\mathbf{q})\times c^\dagger{}_{\mathbf{k}_4\sigma}c^\dagger{}_{\mathbf{k}_3\sigma'}c_{\mathbf{k}_2\sigma'}c_{\mathbf{k}_1\sigma}\times\text{spatial integrals} \tag{4.90}$$

where the spatial integrals take the form

$$\int d^3x d^3x' e^{i(\mathbf{k}_1-\mathbf{k}_4+\mathbf{q})\cdot\mathbf{x}}e^{i(\mathbf{k}_2-\mathbf{k}_3-\mathbf{q})\cdot\mathbf{x}'} = (2\pi)^6\delta^{(3)}(\mathbf{k}_4-\mathbf{k}_1-\mathbf{q})\delta^{(3)}(\mathbf{k}_3-\mathbf{k}_2+\mathbf{q}) \tag{4.91}$$

which impose momentum conservation at each scattering event. Using the spatial integrals to eliminate the integrals over $\mathbf{k}_3$ and $\mathbf{k}_4$, the final result is

$$\hat{V} = \frac{1}{2}\sum_{\sigma\sigma'}\int_{\mathbf{k}_{1,2},\mathbf{q}}\frac{d^3q}{(2\pi)^3}V(\mathbf{q})c^\dagger{}_{\mathbf{k}_1+\mathbf{q}\sigma}c^\dagger{}_{\mathbf{k}_2-\mathbf{q}\sigma'}c_{\mathbf{k}_2\sigma'}c_{\mathbf{k}_1\sigma} \tag{4.92}$$

In other words, when the particles scatter at positions x and x', momentum is conserved. Particle 1 comes in with momentum $\mathbf{k}_1$, and transfers momentum $\mathbf{q}$ to particle 2. Particle 2 comes in with momentum $\mathbf{k}_2$, and thereby gains momentum $\mathbf{q}$:

$$\begin{array}{lll}\text{particle 1} & \mathbf{k}_1 & \rightarrow \quad \mathbf{k}_1+\mathbf{q} \\ \text{particle 2} & \mathbf{k}_2 & \rightarrow \quad \mathbf{k}_2-\mathbf{q}\end{array} \tag{4.93}$$

as illustrated in Fig. 4.1. The matrix element associated with this scattering process is merely the Fourier transform of the potential $V(\mathbf{q})$.

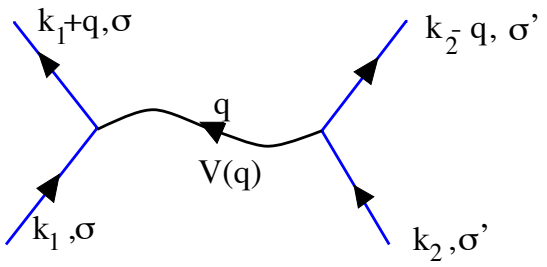


Figure 4.1: Scattering of two particles, showing transfer of momentum. $\mathbf{q}$.

Example 4.4: Particles interact via a delta-function interaction $V(x) = Ua^3\delta^{(3)}(x)$. Write down the second-quantized interaction in a momentum space representation.

Solution: The Fourier transform of the interaction is

$$V(q) = \int d^3x U a^3 \delta(x) e^{-i\mathbf{q}\cdot\mathbf{x}} = Ua^3 \tag{4.94}$$

so the interaction in momentum space is

$$\hat{V} = \sum_{\sigma\sigma'} \frac{Ua^3}{2} \int_{\mathbf{k}_{1,2},\mathbf{q}} \frac{d^3q}{(2\pi)^3} c^\dagger_{\mathbf{k}_1-\mathbf{q}\sigma} c^\dagger_{\mathbf{k}_2+\mathbf{q}\sigma'} c_{\mathbf{k}_2\sigma'} c_{\mathbf{k}_1\sigma} \tag{4.95}$$

Example 4.5: A set of fermions interact via a screened Coulomb (Yukawa) potential

$$V(r) = \frac{Ae^{-\lambda r}}{r} \tag{4.96}$$

Write down the interaction in momentum space.

Solution: The interaction in momentum space is given by

$$\hat{V} = \frac{1}{2} \sum_{\sigma\sigma'} \int_{\mathbf{k}_{1,2},\mathbf{q}} \frac{d^3q}{(2\pi)^3} V(\mathbf{q}) c^\dagger_{\mathbf{k}_1+\mathbf{q}\sigma} c^\dagger_{\mathbf{k}_2-\mathbf{q}\sigma'} c_{\mathbf{k}_2\sigma'} c_{\mathbf{k}_1\sigma} \tag{4.97}$$

where

$$V(\mathbf{q}) = \int d^3x \frac{Ae^{-\lambda r}}{r} e^{-i\mathbf{q}\cdot\mathbf{x}} \tag{4.98}$$

To carry out this integral, we use Polar co-ordinates with the z-axis aligned along the direction $\hat{\mathbf{q}}$. Writing $\mathbf{q}\cdot\mathbf{x} = qr\cos\theta$, then $d^3x = r^2 d\phi d\cos\theta \to 2\pi r^2 d\cos\theta$, so that

$$V(\mathbf{q}) = \int 4\pi r^2 dr V(r) \underbrace{\frac{1}{2}\int_{-1}^{1} d\cos\theta\, e^{-iqr\cos\theta}}_{\langle e^{-i\mathbf{q}\cdot\mathbf{x}}\rangle = \frac{\sin qr}{qr}} \tag{4.99}$$

so that for an arbitrary spherically symmetric potential

$$V(q) = \int_0^\infty 4\pi r^2 dr V(r) \left(\frac{\sin qr}{qr}\right) \tag{4.100}$$

In this case,

$$V(q) = \frac{4\pi A}{q} \int_0^\infty dr e^{-\lambda r} \sin(qr) = \frac{4\pi A}{q^2+\lambda^2}, \tag{4.101}$$

Notice that the Coulomb interaction,

$$V(r) = \frac{e^2}{4\pi\epsilon_0 r}, \tag{4.102}$$

is the infinite range limit of the Yukawa potential, with $\lambda = 0$, $A = e^2/4\pi\epsilon_o$, so that for the Coulomb interaction,

$$V(q) = \frac{e^2}{q^2\epsilon_o}. \tag{4.103}$$

Example 4.6: If one transforms to a new one particle basis, writing $\psi(x) = \sum_s \Phi_s(x) c_s$, show that the interaction becomes

$$\hat{V} = \frac{1}{2} \sum_{lmnp} c^\dagger{}_l c^\dagger{}_m c_n c_p \langle lm|V|pn\rangle \tag{4.104}$$

where

$$\langle lm|V|pn\rangle = \int_{x,x'} \Phi^*_l(x)\Phi_p(x)\Phi^*_m(x')\Phi^*_n(x') V(x-x') \tag{4.105}$$

is the matrix element of the interaction between the two particle states $|lm\rangle$ and $|pn\rangle$.

4.7 Equivalence with the Many Body Schroedinger Equation

In this section, we establish that our second-quantized version of the many body Hamiltonian is indeed equivalent to the many-body Schroedinger equation. Let us start with the Hamiltonian for an interacting gas of charged particles,

$$H = \overbrace{\sum_{\sigma}\int_x \psi_\sigma^\dagger\Big[-\frac{\hbar^2\nabla^2}{2m} + U(x) - \mu\Big]\psi_\sigma(x)}^{H_o} + \overbrace{\frac{1}{2}\sum_{\sigma\sigma'}\int_{x,x'} V(x-x') : \hat\rho(x)\hat\rho(x') :}^{\hat V}. \qquad (4.106)$$

where $\int_x \equiv \int d^3x$, and by convention, we work in the Grand Canonical ensemble, subtracting the term μN from the Schrödinger Hamiltonian H_S, $H = H_S - \mu N$. For a Coulomb interaction

$$V(x-x') = \frac{e^2}{4\pi\epsilon_o|x-x'|} \qquad (4.107)$$

but the interaction might take other forms, such as the hard-core interaction between neutral atoms in liquid He-3 and He-4.

The equation of motion of the field operator is

$$i\hbar\frac{\partial\psi_\sigma}{\partial t} = -[H, \psi_\sigma]. \qquad (4.108)$$

Using the relations

$$\begin{aligned}
[\psi_{\sigma'}^\dagger(x')O_{x'}\psi_{\sigma'}(x'), \psi_\sigma(x)] &= -\delta_{\sigma\sigma'}\delta^3(x-x')O_x\psi_\sigma(x), \\
: [\rho(x_1)\rho(x_2), \psi_\sigma(x)] : &= : [\rho(x_1), \psi_\sigma(x)]\rho(x_2) : + : \rho(x_1)[\rho(x_2), \psi_\sigma(x)] : \\
&= -\delta^3(x_1-x)\rho(x_2)\psi_\sigma(x) - \delta^3(x_2-x)\rho(x_1)\psi_\sigma(x)
\end{aligned}$$

we can see that the comutators of the one- and two-particle parts of the Hamiltonian with the field operator are

$$\begin{aligned}
-[H_o, \psi_\sigma(x)] &= \Big[-\frac{\hbar^2\nabla^2}{2m} + U(x) - \mu\Big]\psi_\sigma(x) \\
-[V, \psi_\sigma(x)] &= \int d^3x' V(x'-x)\rho(x')\psi_\sigma(x)
\end{aligned} \qquad (4.109)$$

The final equation of motion of the field operator thus resembles a one-particle Schrodinger equation.

$$i\hbar\frac{\partial\psi_\sigma}{\partial t} = \Big[-\frac{\hbar^2\nabla^2}{2m} + U(x) - \mu\Big]\psi_\sigma(x) + \int d^3x' V(x'-x)\rho(x')\psi_\sigma(x) \qquad (4.110)$$

If we now apply this to the many body wavefunction, we obtain

$$\begin{aligned}
i\hbar\frac{\partial\Psi(1,2,\ldots N)}{\partial t} &= i\hbar\sum_{r=1,N}\langle 0|\psi(1)\ldots\frac{\partial\psi(r)}{\partial t}\ldots\psi(N)|\Psi\rangle \\
&= \sum_j\Big[-\frac{\hbar^2\nabla_j^2}{2m} + U(x_j) - \mu\Big]\Psi
\end{aligned}$$

$$+ \sum_j\int d^3x' V(x'-x_j)\langle 0|\psi(1)\ldots\rho(x')\psi_\sigma(x_j)\ldots\psi(N)|\Psi\rangle$$

By commuting the density operator to the left, until it annihilates with the vacuum, we find that

$$\langle 0|\psi(1)\ldots\rho(x')\psi_\sigma(x_j)\ldots\psi(N)|\Psi\rangle = \sum_{l<j}\delta^3(x'-x_l)\langle 0|\psi(1)\ldots\psi(N)|\Psi\rangle \qquad (4.111)$$

so that the final expression for the time evolution of the many body wavefunction is precisely the same as we obtain in a first quantized approach.

$$i\hbar\frac{\partial\Psi}{\partial t} = \Big(\sum_j\mathcal{H}_j^{(o)} + \sum_{l<j}V_{jl}\Big)\Psi \qquad (4.112)$$

Our second-quantized approach has the advantage that it builds in the exchange statistics, and it does not need to make an explicit reference to the many body wavefunction.

4.8 Identical Conserved Particles in Thermal Equilibrium

4.8.1 Generalities

By quantizing the particle field, we have been led to a version of quantum mechanics with a vastly expanded Hilbert space which includes the vacuum and all possible states with an arbitrary number of particles. An exactly parallel development occurs in statistical thermodynamics, in making the passage from a canonical, to a grand canonical ensemble, where systems are considered to be in equilibrium with a heat and particle bath. Not surprisingly then, second quantization provides a beautiful way of treating a grand canonical ensemble of identical particles.

When we come to treat conserved particles in thermal equilibrium, we have to take into the account the conservation of two independent quantities

- Energy. E
- Particle number. N

Statistical mechanics usually begins with an ensemble of identical systems of definite particle number and energy E and N respectively. (More precisely, particle number and energy lying in the narrow ranges $[N, N+dN]$ and $[E, E+dE]$, respectively). Such an ensemble is called a "microcanonical ensemble". This is a confusing name, because it suggests something "small", yet typically, a microcanonical ensemble is an ensemble of identical, macroscopic systems that play the role of a heat bath[8, 9, 10, 11]. The ergodic hypothesis of statistical mechanics assumes that in such an ensemble, all accesible quantum states within this narrow band of allowed energies and particle number are equally probable ("*equal à priori probability*").

Now suppose we divide the system into two parts - a vast "heat bath" and a tiny sub-system, exchanging energy and particles, as shown in Fig. 4.2 until they reach a state of thermal equilibrium.

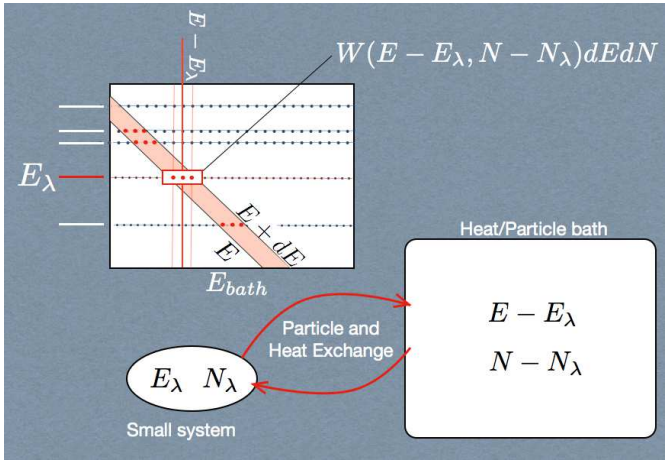


Figure 4.2: Illustrating equilibrium between a small system and a large heat bath. Inset illustrates how the number of states with energy E_λ, particle number N_λ is proportional to the density of states in the big system.

In the vast heat and particle bath, the energy levels are so close together, that they form a continuum. The density of states per unit energy and particle number is taken to be $W(E', N')$, where E' is the energy and N' the number of particles in the bath. When the system is in a quantum state $|\lambda\rangle$ with energy E_λ, particle number N_λ, the large system has energy $E' = E - E_\lambda$, particle number $N' = N - N_\lambda$.

Assuming equal à *priori* probability, the probability that the small system is in state $|\lambda\rangle$ is proportional to the number of states $W(E, N)$ of the heat bath with energy $E - E_\lambda$ and particle number $N - N_\lambda$,

$$p(E_\lambda, N_\lambda) \propto W(E - E_\lambda, N - N_\lambda) = e^{\ln W(E-E_\lambda, N-N_\lambda)}. \tag{4.113}$$

Now following Boltzmann, we can tentatively identify $W(E, N)$ with the entropy $S(E, N)$ of the heat bath, (see exercise 4.4) according to the famous formula

$$S_B(E, N) = k_B \ln W(E, N) \tag{4.114}$$

where we have included the subscript B to delineate the heat bath. It follows that

$$p(E_\lambda, N_\lambda) \propto \exp\left[\frac{1}{k_B} S_B(E - E_\lambda, N - N_\lambda)\right] \tag{4.115}$$

Now E_λ and N_λ are tiny perturbations to the total energy and particle number of the heat bath, so we may approximate $S(E - E_\lambda, N - N_\lambda)$ by a linear expansion,

$$S_B(E - E_\lambda, N - N_\lambda) = S_B(E, N) - E_\lambda \frac{\partial S_B}{\partial E} - N_\lambda \frac{\partial S_B}{\partial N} + \ldots. \tag{4.116}$$

Now according to thermodynamics $dE = TdS + \mu dN$ where T and μ are the temperature and chemical potential, respectively, so that $dS_B = \frac{1}{T}dE - \frac{\mu}{T}dN$, allowing us to identify

$$\begin{aligned} \frac{1}{k_B}\frac{\partial S_B}{\partial E} &= \frac{\partial \ln W}{\partial E} = \frac{1}{k_B T} \equiv \beta, \\ \frac{1}{k_B}\frac{\partial S_B}{\partial N} &= \frac{\partial \ln W}{\partial N} = -\frac{\mu}{k_B T} \equiv -\mu\beta. \end{aligned} \tag{4.117}$$

These are the Lagrange multipliers associated with the conservation of energy and particle number[1]. Once we have made this expansion, it follows that the probability to be in state $|\lambda\rangle$ is

$$p_\lambda = \frac{1}{Z} e^{-\beta(E_\lambda - \mu N_\lambda)}, \tag{4.118}$$

where the normalizing partition function is $Z = \sum_\lambda e^{-\beta(E_\lambda - \mu N_\lambda)}$.

To recast statistical mechanics in the language of many body theory, we need to rewrite the above expression in terms of operators. Let us begin with the partition function, which we may rewrite as

$$\begin{aligned} Z &= \sum_\lambda e^{-\beta(E_\lambda - \mu N_\lambda)} \\ &= \sum_\lambda \langle\lambda| e^{-\beta(\hat{H} - \mu\hat{N})} |\lambda\rangle = \mathrm{Tr}[e^{-\beta(\hat{H} - \mu\hat{N})}]. \end{aligned} \tag{4.119}$$

Although we started with the eigenstates of energy and particle number, the invariance of the trace under unitary transformations ensures that this final expression is independent of the many body basis.

Next, we cast the expectation value $\langle\hat{A}\rangle$ in a basis-independent form. Suppose the quantity A, represented by the operator $\hat{A}$, is diagonal in the basis of energy eigenstates $|\lambda\rangle$, then the expectation value of A in the ensemble is

$$\langle A\rangle = \sum_\lambda p_\lambda \langle\lambda|\hat{A}|\lambda\rangle = \mathrm{Tr}[\hat{\rho}\hat{A}]. \tag{4.120}$$

[1] Incidentally, if you are uncomfortable with the use of classical thermodynamics to identify these quantities in terms of the temperature and chemical potential, you may regard these assignments as tentative, pending calculations of physical properties that allow us to definitively identify them in terms of temperature and chemical potential.

Here we have elevated the probability distribution p_λ to an operator- the Boltzmann density matrix:

$$\hat{\rho} = \sum_\lambda |\lambda\rangle p_\lambda \langle\lambda| = Z^{-1} e^{-\beta(\hat{H}-\mu\hat{N})} \tag{4.121}$$

This derivation of (4.120) assumed that $\hat{A}$ could be simultaneously diagonalized with the energy and particle number. However, quantum statistical mechanics, makes the radical assertion that (4.120) holds for all quantum operators $\hat{A}$ representing observables, *even when the operator $\hat{A}$ does not commute with $\hat{H}$ or $\hat{N}$*, and is thus not diagonal in the energy and particle number basis.

4.8.2 Identification of the Free energy: Key Thermodynamic Properties

There are a number of key thermodynamic quantities of great interest: the energy E, the particle number N, the entropy S and the Free energy $F = E - ST - \mu N$. One of the key relations from elementary thermodynamics is that

$$dE = TdS - \mu dN - PdV \tag{4.122}$$

By putting $F = E - TS - \mu N$, $dF = dE - dTS - SdT - \mu dN - Nd\mu$, one can also derive

$$dF = -SdT - Nd\mu - PdV \tag{4.123}$$

a relationship of great importance.

The energy and particle number can be easily written in the language of second-quantization as

$$\begin{aligned} E &= \mathrm{Tr}[\hat{H}\hat{\rho}], \\ N &= \mathrm{Tr}[\hat{N}\hat{\rho}], \end{aligned} \tag{4.124}$$

but what about the entropy? From statistical mechanics, we know that the general expression for the entropy is given by

$$S = -k_B \sum_\lambda p_\lambda \ln p_\lambda \tag{4.125}$$

Now since the diagonal elements of the density matrix are p_λ, we can rewrite this expression as

$$S = -k_B \mathrm{Tr}[\hat{\rho}\ln\hat{\rho}] \tag{4.126}$$

If we substitute $\ln\hat{\rho} = -\beta(\hat{H} - \mu\hat{N}) - \ln Z$ into this expression, we obtain

$$\begin{aligned} S &= \frac{1}{T}\mathrm{Tr}\hat{\rho}(H - \mu N) + k_B \ln Z \\ &= \frac{1}{T}(E - \mu N) + k_B \ln Z \end{aligned} \tag{4.127}$$

i.e $-k_B T \ln Z = E - ST - \mu N$, from which we identify

$$F = -k_B T \ln Z \tag{4.128}$$

as the Free energy. Summarizing these key relationships all together, we have

Thermodynamic Relations

F	$=$	$-k_B T \ln Z$,	**Free energy**
Z	$=$	$\mathrm{Tr}[e^{-\beta(\hat{H}-\mu\hat{N})}]$,	**Partition function**
$\hat{\rho}$	$=$	$\frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{Z}$,	**Density Matrix**
N	$=$	$\mathrm{Tr}[\hat{N}\hat{\rho}] = -\frac{\partial F}{\partial \mu}$	Particle number
S	$=$	$-k_B \mathrm{Tr}[\hat{\rho}\ln\hat{\rho}] = -\frac{\partial F}{\partial T}$	Entropy
P	$=$	$-\frac{\partial F}{\partial V}$,	Pressure
$E - \mu N$	$=$	$\mathrm{Tr}[(\hat{H} - \mu\hat{N})\hat{\rho}], = -\frac{\partial \ln Z}{\partial \beta}$	Energy

Notice how, in this way, all the key thermodynamic properties can be written as appropriate derivatives of Free energy.

Example 4.7: (i) Enumerate the energy eigenstates of a single fermion Hamiltonian.

$$H = \epsilon c^\dagger c \tag{4.129}$$

where $\{c, c^\dagger\} = 1, \{c,\ c\} = \{c^\dagger,\ c^\dagger\} = 0$.

(ii) Calculate the number of fermions at temperature T.

Solution (i) The states of this problem are the vacuum state and the one-particle state

$$\begin{aligned} |0\rangle \qquad & E = 0, \\ |1\rangle = c^\dagger|0\rangle, \quad & E = \epsilon. \end{aligned} \tag{4.130}$$

(ii) The number of fermions at temperature T is given by

$$\langle\hat{n}\rangle = \mathrm{Tr}[\hat{\rho}\hat{n}] \tag{4.131}$$

where $\hat{n} = c^\dagger c$,

$$\rho = e^{-\beta(\hat{H}-\mu\hat{N})}/Z \tag{4.132}$$

is the density matrix, and where

$$Z = \mathrm{Tr}[e^{-\beta(H-\mu N)}] \tag{4.133}$$

is the "partition function". For this problem, we can write out the matrices explicitly.

$$e^{-\beta H} = \begin{bmatrix} 1 & 0 \\ 0 & e^{-\beta(\epsilon-\mu)} \end{bmatrix}, \qquad \hat{n} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \tag{4.134}$$

so that

$$Z = 1 + e^{-\beta(\epsilon-\mu)} \tag{4.135}$$

and

$$\mathrm{Tr}[\hat{n}e^{-\beta H}] = e^{-\beta(\epsilon-\mu)} \tag{4.136}$$

The final result is thus

$$\langle \hat{n} \rangle = \frac{e^{-\beta(\epsilon-\mu)}}{1 + e^{-\beta(\epsilon-\mu)}} = \frac{1}{e^{\beta(\epsilon-\mu)} + 1} \tag{4.137}$$

which is the famous Fermi-Dirac function for the number of fermions in a state of energy ϵ, chemical potential μ.

4.8.3 Independent Particles

In a system of independent particles with many energy levels, ϵ_λ each energy level can be regarded as an independent member of a microcanonical ensemble. Formally, this is because the Hamiltonian is a sum of independent Hamiltonians

$$H - \mu N = \sum_\lambda (\epsilon_\lambda - \mu)\hat{n}_\lambda \tag{4.138}$$

so that the partition function is then a product of the individual partition functions:

$$Z = \mathrm{Tr}[\prod_{\lambda\,\otimes} e^{-\beta(\epsilon_\lambda-\mu)\hat{n}_\lambda}] \tag{4.139}$$

and since the trace of an (exterior) product of matrices, is equal to the product of their individual traces, ($\mathrm{Tr}\prod_{\lambda\otimes} = \prod_\lambda \mathrm{Tr}$),

$$Z = \prod_\lambda \mathrm{Tr}[e^{-\beta(\epsilon_\lambda-\mu)\hat{n}_\lambda}] = \prod_\lambda Z_\lambda \tag{4.140}$$

Since

$$Z_\lambda = \begin{cases} 1 + e^{-\beta(\epsilon_\lambda-\mu)} & \textit{Fermions} \\ 1 + e^{-\beta(\epsilon_\lambda-\mu)} + e^{-2\beta(\epsilon_\lambda-\mu)} + \ldots = (1 - e^{-\beta(\epsilon_\lambda-\mu)})^{-1} & \textit{Bosons} \end{cases} \tag{4.141}$$

The corresponding Free energy is given by

$$F = \mp k_B T \sum_\lambda \ln[1 \pm e^{-\beta(\epsilon_\lambda-\mu)}], \qquad \begin{cases} fermions \\ bosons \end{cases} \tag{4.142}$$

The occupancy of the l th level is independent of all the other levels, and given by

$$\begin{aligned} \langle \hat{n}_l \rangle = \mathrm{Tr}[\hat{\rho}\hat{n}_l] &= \mathrm{Tr}[(\prod_{\otimes} \hat{\rho}_\lambda)\hat{n}_l] \\ &= \prod_{\lambda\neq l} \overbrace{\mathrm{Tr}[\rho_\lambda]}^{=1} \times \mathrm{Tr}[\rho_l \hat{n}_l] = \frac{1}{e^{\beta(\epsilon_l-\mu)} \pm 1} \end{aligned} \tag{4.143}$$

where (+) refers to Fermions and (−) to bosons.

In the next chapter, we shall examine the consequences of these relationships.

4.9 Exercises

1. In this question $c_i^\dagger$ and c_i are fermion creation and annihilation operators and the states are fermion states. Use the convention

   $|11111000\ldots\rangle = c_5^\dagger c_4^\dagger c_3^\dagger c_2^\dagger c_1^\dagger |\mathrm{vacuum}\rangle$.

   (a) Evaluate $c_3^\dagger c_6 c_4 c_6^\dagger c_3 |111111000\ldots\rangle$.

   (b) Write $|1101100100\ldots\rangle$ in terms of excitations about the "filled Fermi sea" $|1111100000\ldots\rangle$. Interpret your answer in terms of electron and hole excitations.

   (c) Find $\langle\psi|\hat{N}|\psi\rangle$ where $|\psi\rangle = A|100\rangle + B|111000\rangle$, $\hat{N} = \sum_i c_i^\dagger c_i$.

2. (a) (a) Consider two fermions, a_1 and a_2. Show that the Boguilubov transformation

   $$\begin{aligned} c_1 &= u a_1 + v a_2^\dagger \\ c_2^\dagger &= -v a_1 + u a_2^\dagger \end{aligned} \tag{4.144}$$

   where u and v are real, preserves the canonical anti-commutation relations if $u^2 + v^2 = 1$.

   (b) Use this result to show that the Hamiltonian

   $$H = \epsilon(a_1^\dagger a_1 - a_2 a_2^\dagger) + \Delta(a_1^\dagger a_2^\dagger + \mathrm{H.c.}) \tag{4.145}$$

   can be diagonalized in the form

   $$H = \sqrt{\epsilon^2 + \Delta^2}(c_1^\dagger c_1 + c_2^\dagger c_2 - 1) \tag{4.146}$$

   (c) What is the ground-state energy of this Hamiltonian?

   (d) Write out the ground-state wavefunction in terms of the original operators $c_1^\dagger$ and $c_2^\dagger$ and their corresponding vacuum $|0\rangle$, $(c_{1,2}|0\rangle = 0)$.

3. Consider a system of fermions or bosons, created by the field $\psi^\dagger(\mathbf{r})$ interacting under the potential

   $$V(r) = \begin{cases} U, & (r < R), \\ 0, & (r > R), \end{cases} \tag{4.147}$$

   (a) Write the interaction in second quantized form.

(b) Switch to the momentum basis, where $\psi(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} c_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$. Verify that $[c_{\mathbf{k}},\ c^\dagger_{\mathbf{k}'}]_\pm = (2\pi)^3\delta^{(3)}(\mathbf{k}-\mathbf{k}')$ and write the interaction in this new basis. Please sketch the form of the interaction in momentum space.

4. (a) Show that for a general system of conserved particles at chemical potential, the total particle number in thermal equilibrium can be written as

$$N = -\partial F/\partial\mu \tag{4.148}$$

where

$$\begin{aligned} F &= -k_B T \ln Z \\ Z &= \mathrm{Tr}[e^{-\beta(\hat{H}-\mu N)}]. \end{aligned} \tag{4.149}$$

(b) Apply this to a single bosonic energy level, where

$$H - \mu N = (\epsilon - \mu)a^\dagger a \tag{4.150}$$

and $\hat{a}^\dagger$ creates either a Fermion, or a boson, to show that

$$\langle \hat{n} \rangle = \frac{1}{e^{\beta(\epsilon-\mu)} - 1} \tag{4.151}$$

Why does μ have to be negative positive for bosons?

5. (Equivalence of the microcanonical and Gibb's ensembles for large systems.)
In a microcanonical ensemble, the density matrix can be given by

$$\hat{\rho}_M = \frac{1}{W}\delta(E - \hat{H})\delta(N - \hat{N})$$

where E and N are the energy and particle number respectively, while

$$W \equiv W(E,N) = \mathrm{Tr}\left[\delta(E - \hat{H})\delta(N - \hat{N})\right]$$

is the "density of states" at energy E, particle number N. This normalizing quantity plays a role similar to the partition function in the Gibb's ensemble.

(a) By rewriting the delta functions inside the above trace W as an inverse Laplace transforms, such as

$$\delta(x - \hat{H}) = \int_{\beta_0 - i\infty}^{\beta_0 + i\infty} \frac{d\beta}{2\pi i} e^{-\beta(x-\hat{H})},$$

and evaluating the resulting integrals at the saddle point of the integrand, show that for a large system W is related to the entropy by Boltzmann's relation

$$S(E,N) = k_B \ln W(E,N).$$

(b) Using your results, show that in a large system, the expectation value of an operator is the same for corresponding Gibb's and microcanonical ensembles, namely

$$\langle A \rangle = \mathrm{Tr}[\rho_M \hat{A}] = \mathrm{Tr}[\rho_B \hat{A}]$$

where $\hat{\rho}_B = Z^{-1} e^{-\beta(H-\mu\hat{N})}|_{\beta=\beta_0,\mu=\mu_0}$ is the Boltzmann density matrix evaluated at the saddle point values of β_0 and μ_0,

$$\beta_0 = \frac{\partial \ln W}{\partial E}, \qquad \mu_0 = \beta_0^{-1}\frac{\partial \ln W}{\partial N}.$$

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Chapter 5

Simple Examples of Second-quantization

In this section, we give three examples of the application of second quantization, mainly to non-interacting systems.

5.1 Jordan Wigner Transformation

A "non-interacting" gas of Fermions is still highly correlated: the exclusion principle introduces a "hard-core" interaction between fermions in the same quantum state. This feature is exploited in the Jordan -Wigner representation of spins. A classical spin is represented by a vector pointing in a specific direction. Such a representation is fine for quantum spins with extremely large spin S, but once the spin S becomes small, spins behave as very new kinds of object. Now their spin becomes a quantum variable, subject to its own zero-point motions. Furthermore, the spectrum of excitations becomes discrete or grainy.

Quantum spins are notoriously difficult objects to deal with in many-body physics, because they do not behave as canonical fermions or bosons. In one dimension however, it turns out that spins with $S = 1/2$ actually behave like fermions. We shall show this by writing the quantum spin-1/2 Heisenberg chain as an interacting one dimensional gas of fermions, and we shall actually solve the limiting case of the one-dimensional spin-1/2 x-y model.

Jordan and Wigner observed[1] that the down and up state of a single spin can be thought of as an empty or singly occupied fermion state, (Fig. 5.1.) enabling them to make the mapping

$$|\uparrow\rangle \equiv f^\dagger|0\rangle, \qquad |\downarrow\rangle \equiv |0\rangle. \tag{5.1}$$

.

An explicit representation of the spin raising and lowering operators is then

$$\begin{aligned} S^+ &= f^\dagger = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \\ S^- &= f \equiv \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \end{aligned} \tag{5.2}$$

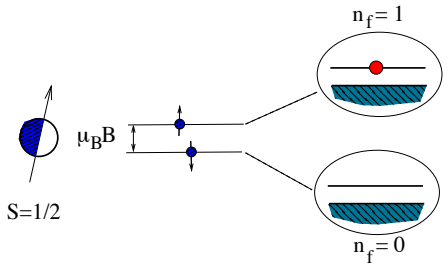

Figure 5.1: Showing how the "up" and "down" states of a spin-1/2 can be treated as a one particle state which is either full, or empty.

The z component of the spin operator can be written

$$S_z = \frac{1}{2}\Big[|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|\Big] \equiv f^\dagger f - \frac{1}{2} \tag{5.3}$$

We can also reconstruct the transverse spin operators,

$$\begin{aligned} S_x &= \frac{1}{2}(S^+ + S^-) = \frac{1}{2}(f^\dagger + f), \\ S_y &= \frac{1}{2i}(S^+ - S^-) = \frac{1}{2i}(f^\dagger - f), \end{aligned} \tag{5.4}$$

The explicit matrix representation of these operators makes it clear that they satisfy the same algebra

$$[S_a, S_b] = i\epsilon_{abc}S_c. \tag{5.5}$$

Curiously, due to a hidden supersymmetry, they also satisfy an anti-commuting algebra

$$\{S_a, S_b\} = \frac{1}{4}\{\sigma_a, \sigma_b\} = \frac{1}{2}\delta_{ab}, \tag{5.6}$$

and in this way, the Pauli spin operators provided Jordan and Wigner with an elementary model of a fermion.

Unfortunately the represeentation needs to be modified if there is more than one spin, for independent spin operators commute, but independent fermions anticommute! Jordan and Wigner discovered a way to fix up this difficulty in one dimension by attaching a phase factor called a "string" to the fermions[1]. For a chain of spins in one dimension, the Jordan Wigner representation of the spin operator at site j is defined as

$$S_j^+ = f_j^\dagger e^{i\phi_j} \tag{5.7}$$

where the phase operator ϕ_j contains the sum over all fermion occupancies at sites to the left of j,

$$\phi_j = \pi \sum_{l<j} n_j \tag{5.8}$$

The operator $e^{i\hat{\phi}_j}$ is known as a "string operator".

The complete transformation is then

$$\left.\begin{array}{rcl} S^z_j &=& f^\dagger{}_j f_j - \frac{1}{2}, \\ S^+_j &=& f^\dagger{}_j e^{i\pi \sum_{l<j} n_l}, \\ S^-_j &=& f_j e^{-i\pi \sum_{l<j} n_l} \end{array}\right\} \textbf{Jordan Wigner transformation} \tag{5.9}$$

(Notice $e^{i\pi n_j} = e^{-i\pi n_j}$ is a Hermitian operator so that overall sign of the phase factors can be reversed without changing the spin operator.) In words:

$$\text{Spin} = \text{Fermion} \times \text{string}.$$

The important property of the string, is that it *anticommutes* with any fermion operator to the left of its free end. To see this, note first that is that the operator $e^{i\pi n_j}$ *anticommutes* with the fermion operator f_j. This follows because f_j reduces n_j from unity to zero, so that $f_j\, e^{i\pi n_j} = -f_j$ whereas $e^{i\pi n_j}\, f_j = f_j$. from which it follows that

$$\{e^{i\pi n_j}, f_j\} = e^{i\pi n_j} f_j + f e^{i\pi n_j} = f_j - f_j = 0 \tag{5.10}$$

and similarly, from the conjugate of this expression $\{e^{i\pi n_j}, f^\dagger{}_j\} = 0$. Now the phase factor $e^{i\pi n_l}$ at any other site $l \neq j$ commutes with f_j and $f^\dagger_j$, so that the string operator $e^{i\hat{\phi}_j}$ anticommutes with all fermions at all sites to the "left" of j $l < j$:

$$\{e^{i\phi_j}, f^{(\dagger)}_l\} = 0, \qquad (l < k)$$

whilst commuting with fermions at all other sites $l \geq j$,

$$[e^{i\phi_j}, f^{(\dagger)}_l] = 0, \qquad (l \geq k).$$

We now can verify that the transverse spin operators satisfy the correct commutation algebra. Suppose $j < k$, then $e^{i\phi_j}$ commutes with fermions at site j and k so that

$$[S^{(\pm)}_j, S^{(\pm)}_k] = [f^{(\dagger)}_j e^{i\phi_j}, f^{(\dagger)}_k e^{i\phi_k}] = e^{i\phi_j}[f^{(\dagger)}_j, f^{(\dagger)}_k e^{i\phi_k}]$$

But $f^{(\dagger)}_j$ antcommutes with both $f^{(\dagger)}_k$ and $e^{i\pi\phi_k}$ so it commutes with their product $f^{(\dagger)}_k e^{i\phi_k}]$, and hence

$$[S^{(\pm)}_j, S^{(\pm)}_k] \propto [f^{(\dagger)}_j, f^{(\dagger)}_k e^{i\phi_k}] = 0. \tag{5.11}$$

So in this way, we see that by multiplying a fermion by the string operator, it is transformed into a kind of boson.

As an example of the application of this method, we shall now discuss the one-dimensional Heisenberg model

$$H = -J \sum [S^x_j S^x_{j+1} + S^y_j S^y_{j+1}] - J_z \sum_j S^z_j S^z_{j+1} \tag{5.12}$$

In real magnetic systems, local moments can interact via ferromagnetic, or antiferromagnetic interactions. Ferromagnetic interactions generally arise as a result of "direct exchange" in which the Coulomb repulsion energy is lowered when electrons are in a triplet state, because the wavefunction is then spatially antisymmetric. Antiferromagnetic interactions are generally produced by the mechanism of "double exchange", in which electrons on neighbouring sites that form singlets ("antiparallel spin") lower their energy through virtual virtual quantum fluctuations into high energy states in which they occupy the same orbital. Here we have written the model as if the interactions are ferromagnetic.

For convenience, the model can be rewritten as

$$H = -\frac{J}{2} \sum [S^+_{j+1} S^-_j + \text{H.c}] - J_z \sum_j S^z_j S^z_{j+1} \tag{5.13}$$

To fermionize the first term, we note that all terms in the strings cancel, except for a $e^{i\pi n_j}$ which has no effect,

$$\frac{J}{2} \sum_j S^+_{j+1} S^-_j = \frac{J}{2} \sum_j f_{j+1}{}^\dagger e^{i\pi n_j} f_j = \frac{J}{2} \sum_j f_{j+1}{}^\dagger f_j \tag{5.14}$$

so that the transverse component of the interaction induces a "hopping" term in the fermionized Hamiltonian. Notice that the string terms would enter if the spin interaction involved next-nearest neighbors. The z-component of the Hamiltonian becomes

$$-J_z \sum_j S^z_{j+1} S^z_j \;=\; -J_z \sum_j (n_{j+1} - \frac{1}{2})(n_j - \frac{1}{2}) \tag{5.15}$$

Notice how the Ferromagnetic interaction means that spin-fermions attract one-another. The transformed Hamiltonian is then

$$H = -\frac{J}{2} \sum_j (f^\dagger{}_{j+1} f_j + f^\dagger{}_j f_{j+1}) + J_z \sum_j n_j - J_z \sum_j n_j n_{j+1}. \tag{5.16}$$

Interestingly enough, the pure x-y model has no interaction term in it, so this this case can be mapped onto a non-interacting fermion problem, a discovery made by Lieb, Schulz and Mattis in 1961[2].

To write out the fermionized Hamiltonian in its most compact form, let us transform to momentum space, writing

$$f_j = \frac{1}{\sqrt{N}} \sum_k s_k e^{ikR_j} \tag{5.17}$$

where $s^\dagger_k$ creates a spin excitation in momentum space, with momentum k. In this case, the one-particle terms become

$$\begin{aligned} J_z \sum_j n_j &= J_z \sum_k s^\dagger_k s_k. \\ -\frac{J}{2}\sum_j (f^\dagger{}_{j+1} f_j + \text{H.c}) &= -\frac{J}{2N}\sum_k (e^{-ika} + e^{ika}) s^\dagger_k s_{k'} \overbrace{\sum_j e^{-i(k-k')R_j}}^{N\delta_{kk'}} \\ &= -J\sum_k \cos(ka) s^\dagger_k s_k. \end{aligned} \tag{5.18}$$

The anisotropic Heisenberg Hamiltonian can thus be written

$$H = \sum_k \omega_k s^\dagger_k s_k - J_z \sum_j n_j n_{j+1} \tag{5.19}$$

where

$$\omega_k = (J_z - J\cos ka) \tag{5.20}$$

defines a magnon excitation energy, and the second interaction term is still written in the position basis. We can easily cast the second-term in momentum space, by noticing that the interaction is a function of $i-j$ which is $-J_z/2$ for $i-j = \pm 1$ but zero otherwise.The Fourier transform of this short-range interaction is $V(q) = -J_z \cos qa$, so that Fourier transforming the interaction term gives

$$H = \sum_k \omega_k s^\dagger_k s_k - \frac{J_z}{N_s}\sum_{k,k',q} \cos(qa)\; s^\dagger_{k-q} s^\dagger_{k'+q} s_{k'} s_k. \tag{5.21}$$

This transformation holds for both the ferromagnet and antiferromagnet. In the former case, the fermionic spin excitations correspond to the magnons of the ferromagnet. In the latter case, the fermionic spin excitations are often called "spinons".

To see what this Hamiltonian means, let us first neglect the interactions. This is a reasonable thing to do in the limiting cases of (i) the Heisenberg Ferromagnet, $J_z = J$ and (ii) the x-y model $J_z = 0$.

- *Heisenberg Ferromagnet*. $J_z = J$

  In this case, the spectrum

  $$\omega_k = 2J\sin^2(ka/2) \tag{5.22}$$

  is always positive, so that there are no magnons present in the ground-state. The ground-state thus contains no magnons, and can be written

  $$|0\rangle = |\downarrow\downarrow\downarrow \ldots\rangle \tag{5.23}$$

  corresponding to a state with a spontaneous magnetization $M = -N_s/2$.

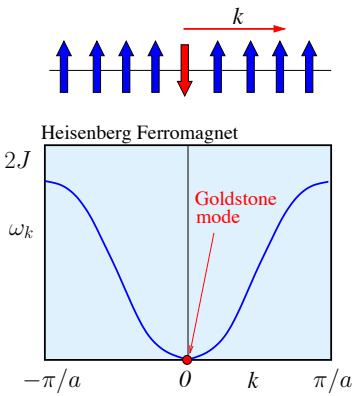

Figure 5.2: Excitation spectrum of the one dimensional Heisenberg Ferromagnet.

Curiously, since $\omega_{k=0} = 0$, it costs no energy to add a magnon of arbitrarily long wavelength. This is an example of a Goldstone mode, and the reason it arises, is because the spontaneous magnetization could actually point in any direction. Suppose we want to rotate the magnetization through an infinitesimal angle $\delta\theta$ about the x axis, then the new state is given by

$$\begin{aligned} |\psi\rangle' &= e^{i\delta\theta S_x}|\downarrow\downarrow\ldots\rangle \\ &= |\downarrow\downarrow\ldots\rangle + i\frac{\delta\theta}{2}\sum_j S^+_j|\downarrow\downarrow\ldots\rangle + O(\delta\theta^2) \end{aligned} \tag{5.24}$$

The change in the wavefunction is proportional to the state

$$\begin{aligned} S^+_{TOT}|\downarrow\downarrow\ldots\rangle &\equiv \sum_j f_j^\dagger e^{i\phi_j}|0\rangle \\ &= \sum_j f_j^\dagger|0\rangle = \sqrt{N_s}s^\dagger_{k=0}|0\rangle \end{aligned} \tag{5.25}$$

In otherwords, the action of adding a single magnon at $q = 0$, rotates the magnetization infinitesimally upwards. Rotating the magnetization should cost no energy, and this is the reason why the $k = 0$ magnon is a zero energy excitation.

- *x-y Ferromagnet*. As J_z is reduced from J, the spectrum develops a negative part, and magnon states with negative energy will become occupied. For the pure $x-y$ model, where $J_z = 0$, the interaction identically vanishes, and the excitation spectrum of the magnons is given by $\omega_k = -J\cos ka$ as sketched in Fig. 5.3. All the negative energy fermion states with $|k| < \pi/2a$

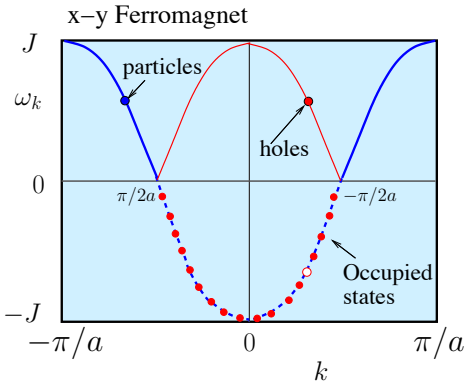

Figure 5.3: Excitation spectrum of the one dimensional x-y Ferromagnet, showing how the negative energy states are filled, the negative energy dispersion curve is "folded over" to describe the positive hole excitation energy.

are occupied, so the ground-state is given by

$$|\Psi_g\rangle = \prod_{|k|<\pi/2a} s^\dagger{}_k|0\rangle \tag{5.26}$$

The band of magnon states is thus precisely half-filled, so that

$$\langle S_z\rangle = \langle n_f - \frac{1}{2}\rangle = 0 \tag{5.27}$$

so that remarkably, there is no ground-state magnetization. We may interpret this loss of ground-state magnetization as a consequence of the growth of quantum spin fluctuations in going from the Heisenberg, to the x-y ferromagnet.

Excitations of the ground-state can be made, either by adding a magnon at wavevectors $|k| > \pi/2a$, or by annihilating a magnon at wavevectors $|k| < \pi/2a$, to form a "hole". The energy to form a hole is $-\omega_k$. To represent the hole excitations, we make a "particle-hole" transformation for the occupied states, writing

$$\tilde{s}_k = \begin{cases} s_k, & (|k| > \pi/2a), \\ s^\dagger_{-k}, & (|k| < \pi/2a) \end{cases} \tag{5.28}$$

These are the "physical" excitation operators. Since $s^\dagger{}_k s_k = 1 - s_k s^\dagger{}_k$, the Hamiltonian of the

pure x-y ferromagnet can be written

$$H_{xy} = \sum_k J|\cos ka|(\tilde{s}^\dagger{}_k\tilde{s}_k - \frac{1}{2}) \tag{5.29}$$

Notice that unlike the pure Ferromagnet, the magnon excitation spectrum is now linear. The ground-state energy is evidently

$$\begin{aligned} E_g &= -\frac{1}{2}\sum_k J|\cos ka| \\ &= -\frac{a}{2}\int_{-\pi/2a}^{\pi/2a}\frac{dk}{2\pi}J\cos(ka) = -\frac{J}{\pi}. \end{aligned} \tag{5.30}$$

But if there is no magnetization, why are there zero-energy magnon modes at $q = \pm\pi/a$? Although there is no true long-range order, it turns out that the spin-correlations in the x-y model display power-law correlations with an infinite spin correlation length, generated by the gapless magnons in the vicinity of $q = \pm\pi/a$.

5.2 The Hubbard Model

In real electronic systems, such as a metallic crystal at first sight it might appear to be a task of hopeless complexity to model the behavior of the electron fluid. Fortunately, even in complex systems, at low energies only a certain subset of the electronic degrees of freedom are excited. This philosophy is closely tied up with the idea of renormalization- the idea that the high energy degrees of freedom in a system can be successively eliminated or "integrated out" to reveal an effective Hamiltonian that describes the important low energy physics. One such model, which has enjoyed great success, is the Hubbard model, first introduced in the early sixties by Hubbard, Gutzwiller and Kanamori[3, 4**?**].

Suppose we have a lattice of atoms where electrons are almost localized in atomic orbitals at each site. In this case, we can use a basis of atomic orbitals. The operator which creates a particle at site j is

$$c^\dagger{}_{j\sigma} = \int d^3x\Phi(\mathbf{x} - \mathbf{R}_j)\psi^\dagger(x)_\sigma \tag{5.31}$$

where $\Phi(\mathbf{x})$ is the wavefunction of a particle in the localized atomic orbital. In this basis, the Hamiltonian governing the motion, and interactions between the particles can be written quite generally as

$$H = \sum_{i,j}\langle i|H_o|j\rangle c^\dagger{}_{i\sigma}c_{j\sigma} + \frac{1}{2}\sum_{lmnp}\langle lm|V|pn\rangle c^\dagger{}_{l\sigma}c^\dagger{}_{m\sigma'}c_{n\sigma'}c_{p\sigma} \tag{5.32}$$

where $\langle i|H_o|j\rangle$ is the one-particle matrix element between states i and j, and $\langle lm|V|pn\rangle$ is the interaction matrix element between two-particle states $|lm\rangle$ and $|pn\rangle$.

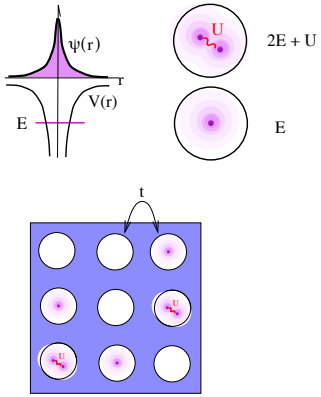

Figure 5.4: Illustrating the Hubbard Model. When two electrons of opposite spin occupy a single atom, this gives rise to a Coulomb repulsion energy U. The amplitude to hop from site to site in the crystal is t.

Let us suppose that the energy of an electron in this state is ϵ. If this orbital is highly localized, then the amplitude for it to tunnel or "hop" between sites will decay exponentially with distance between sites, and to a good approximation, we can eliminate all but the nearest neighbor hopping. In this case, the one-particle matrix elements which govern the motion of electrons between sites are then

$$\langle j|H^{(o)}|i\rangle = \begin{cases} \epsilon & j = i \\ -t & \text{i, j nearest neighbors} \\ 0 & \text{otherwise} \end{cases} \tag{5.33}$$

The hopping matrix element between neigboring states will generally be given by an overlap integral of the wavefunctions with the negative crystalline potential, and for this reason, it is taken to be be negative. Now the matrix element of the interaction between electrons at different sites will be given by

$$\langle lm|V|pn\rangle = \int_{x,x'} \Phi_l^*(x)\Phi_p(x)\Phi_m^*(x')\Phi_n^*(x')V(x-x'), \tag{5.34}$$

but in practice, if the states are well localized, this will be dominated by the onsite interaction between two electrons in a single orbital, so that we may approximate

$$\langle lm|V|pn\rangle = \begin{cases} U & l = p = m = n \\ 0 & \text{otherwise} \end{cases} \tag{5.35}$$

In this situation, the interaction term in (5.32) simplifies to

$$\frac{U}{2}\sum_{j,\sigma\sigma'} c^\dagger{}_{j\sigma}c^\dagger{}_{j\sigma'}c_{j\sigma'}c_{j\sigma} = U\sum_j n_{j\uparrow}n_{j\downarrow}, \tag{5.36}$$

where the exclusion principle ($c^2_{j\sigma} = 0$) means that the interaction term vanishes unless σ σ' are opposite spins. The Hubbard model can be thus be written

$$H = -t\sum_{j,\hat{a},\sigma}[c^\dagger{}_{j+\hat{a}\sigma}c_{j\sigma} + \text{H.c}] + \epsilon\sum_{j\sigma} c^\dagger{}_{j\sigma}c_{j\sigma} + U\sum_j n_{j\uparrow}n_{j\downarrow}, \tag{5.37}$$

where $n_{j\sigma} = c^\dagger{}_{j\sigma}c_{j\sigma}$ represents the number of electrons of spin σ at site j. For completeness, let us rewrite this in momentum space, putting

$$c_{j\sigma} = \frac{1}{\sqrt{N_s}}\sum_{\mathbf{k}} c_{\mathbf{k}\sigma}e^{i\mathbf{k}\cdot\mathbf{R}_j} \tag{5.38}$$

whereupon

$$H = \sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}c^\dagger{}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \frac{U}{N_s}\sum_{\mathbf{q},\mathbf{k},\mathbf{k}'} c^\dagger{}_{\mathbf{k}-\mathbf{q}\uparrow}c^\dagger{}_{\mathbf{k}'+\mathbf{q}\downarrow}c_{\mathbf{k}'\downarrow}c_{\mathbf{k}\uparrow} \tag{5.39}$$

Hubbard model

where

$$\begin{aligned}\epsilon_{\mathbf{k}} &= \sum_i \langle j + \mathbf{R}_i|H_o|j\rangle e^{i\mathbf{k}\cdot\mathbf{R}_i} \\ &= -2t(\cos k_x + \cos k_y + \cos k_z) + \epsilon\end{aligned} \tag{5.40}$$

is recognized as the kinetic energy of the electron excitations which results from their *coherent* hopping motion from site to site. We see that the Hubbard model describes a band of electrons with kinetic energy $\epsilon_{\mathbf{k}}$, and a momentum independent "point" interaction of strength U between particles of opposite spin.

Remark

- This model has played a central part in the theory of magnetism, metal-insulator transitions, and most recently, in the description of electron motion in high temperature superconductors. With the exception of one dimensional physics, we do not, as yet have a complete understanding of the physics that this model can give rise to. One prediction of the Hubbard model which is established, is that under certain circumstance, if interactions become too large the electrons become localized to form what is called "Mott insulator". This typically occurs when the interactions are large and the number of electrons per site is close to one. What is very unclear at the present time, is what happens to the Mott insulator when it is doped, and there are many who believe that a complete understanding of the doped Mott insulator will enable us to understand high temperature superconductivity.

5.3 Non-interacting particles in thermal equilibrium

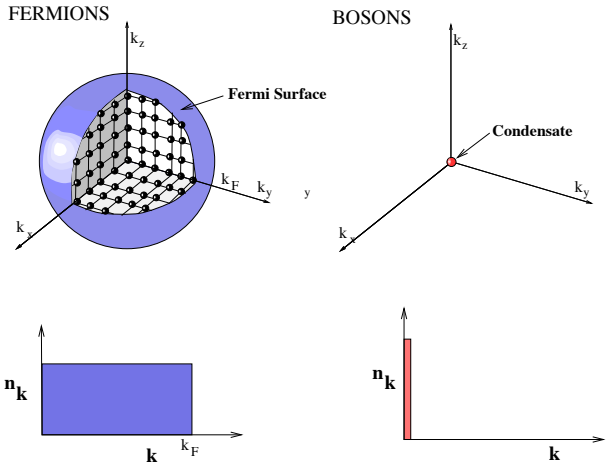

Figure 5.5: Contrasting the ground-states of non-interacting Fermions and non-interacting Bosons. Fermions form a degenerate Fermi gas, with all one-particle states below the Fermi energy individually occupied. Bosons form a Bose Einstein condensate, with a macroscopic number of bosons in the zero momentum state.

Before we start to consider the physics of the interacting problem, let us go back and look at the ground-state properties of free particles. What is not commonly recognized, is that the ground-state of non-interacting, but identical particles is in fact, a highly correlated many body state. For this reason, the non-interacting ground-state has a robustness that does not exist in its classical counterpart. In the next chapter, we shall embody some of these thoughts in by considering the action of turning on the interactions adiabatically. For the moment however, we shall content ourselves with looking at a few of the ground-state properties of non-interacting gases of identical particles.

In practice, quantum effects will influence a fluid of identical particles at the point where their characteristic wavelength is comparable with the separation between particles. At a temperature T the rms momentum of particles is given by $p^2_{RMS} = 3mk_BT$, so that characteristic de Broglie wavelength is given by

$$\lambda_T = \frac{h}{\sqrt{p^2_{RMS}}} = \frac{h}{\sqrt{3mk_BT}} \tag{5.41}$$

so that when $\lambda_T \sim \rho^{-1/3}$, the characteristic temperature is of order

$$k_BT^* \sim \frac{\hbar^2\rho^{2/3}}{2m} \tag{5.42}$$

Below this temperature, identical particles start to interfere with one-another, and a quantum-mechanical treatment of the fluid becomes necessary. In a Fermi fluid, exclusion statistics tends to keep particles apart, enhancing the pressure, whereas for a Bose fluid, the correlated motion of particles in the condensate tends to lower the pressure, ultimately causing it to vanish at the Bose Einstein condensation temperature. In electron fluids inside materials, this characteristic temperature is two orders of magnitude larger than room temperature, which makes the electricity one of the most dramatic examples of quantum physics in everyday phenomena!

5.3.1 Fluid of non-interacting Fermions

The thermodynamics of a fluid of fermions leads to the concept of a "degenerate Fermi liquid", and it is important in a wide range of physical situations, such as

- The ground-state and excitations of metals.
- The low energy physics of liquid Helium 3.
- The degenerate Fermi gas of neutrons, electrons and protons that lies within a neutron star.

The basic physics of each of these cases, can to a first approximation be described by a fluid of non-interacting Fermions, with Hamiltonian

$$H = H_S - \mu N = \sum_{\sigma}(E_{\mathbf{k}} - \mu)c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} \tag{5.43}$$

Following the general discussion of the last section, the Free energy of such a fluid of fermions is is described by a single Free energy functional

$$\begin{aligned} F &= -k_BT\sum_{\mathbf{k}\sigma}\ln[1 + e^{-\beta(E_{\mathbf{k}}-\mu)}] \\ &= -2k_BTV\int_{\mathbf{k}}\ln[1 + e^{-\beta(E_{\mathbf{k}}-\mu)}] \end{aligned} \tag{5.44}$$

where we have taken the thermodnamic limit, replacing $\sum_{\mathbf{k}\sigma} \to 2V\int_{\mathbf{k}}$. By differentiating F with respect to volume, temperature and chemical potential, we can immediately derive the pressure, entropy and particle density of this fluid. Let us however, begin with a more physical discussion.

In thermal equilibrium the number of fermions in a state with momentum $\mathbf{p} = \hbar\mathbf{k}$ is

$$n_{\mathbf{k}} = f(E_{\mathbf{k}} - \mu) \tag{5.45}$$

where

$$f(x) = \frac{1}{e^{\beta x} + 1} \tag{5.46}$$

is the Fermi-Dirac function. At low temperatures, this function resembles a step, with a jump in occupancy spread over an energy range of order k_BT around the chemical potential. At absolute zero $f(x) \to \theta(-x)$, so that the occupancy of each state is given by

$$n_{\mathbf{k}} = \theta(\mu - E_{\mathbf{k}}) \tag{5.47}$$

is a step function with an abrupt change in occupation when $\epsilon = \mu$, corresponding to the fact that states with $E_{\mathbf{k}} < \mu$, are completely occupied, and states above this energy are empty. The zero-temperature value of the chemical potential is often called the "Fermi energy". In momentum space, the occupied states form a sphere, whose radius in momentum space, k_F is often refered to as the Fermi momentum.

The ground-state corresponds to a state where all fermion states with momentum $k < k_F$ are occupied:

$$|\psi_g\rangle = \prod_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma}|0\rangle \tag{5.48}$$

Excitations above this ground-state are produced by the addition of particles at energies above the Fermi wavevector, or the creation of *holes* beneath the Fermi wavevector. To describe these excitations, we make the following *particle-hole* transformation

$$a^\dagger_{\mathbf{k}\sigma} = \begin{cases} c^\dagger_{\mathbf{k}\sigma} & (k > k_F) \quad \text{particle} \\ \sigma c_{-\mathbf{k}-\sigma} & (k > k_F) \quad \text{hole} \end{cases} \tag{5.49}$$

Beneath the Fermi surface, we must replace $c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} \to 1 - a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}$, so that in terms of particle and hole excitations, the Hamiltonian can be re-written

$$H - \mu N = \sum_{\mathbf{k}\sigma} |(E_{\mathbf{k}} - \mu)|a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma} + F_g \tag{5.50}$$

where respectively,

$$F_g = \sum_{|\mathbf{k}|<k_F,\sigma} (E_{\mathbf{k}} - \mu) = 2V \int_{|\mathbf{k}|<k_F} (E_{\mathbf{k}} - \mu), \tag{5.51}$$

is the ground-state Free energy, and E_g and N are the ground-state energy and particle number Notice that

- To create a hole with momentum $\mathbf{k}$ and spin σ, we must destroy a fermion with momentum $-\mathbf{k}$ and spin $-\sigma$. (The additional multiplying factor of σ in the hole definition is a technical feature, required so that the particle and holes have the same spin operators.)

- The excitation energy of a particle or hole is given by $\epsilon^*_{\mathbf{k}} = |E_{\mathbf{k}} - \mu|$, corresponding to "reflecting" the excitation spectrum of the negative energy fermions about the Fermi energy.

The ground-state density of a Fermi gas is given by the volume of the Fermi surface, as follows

$$\langle\hat{\rho}\rangle = \frac{1}{V}\sum_{\mathbf{k}\sigma}\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle = 2\int_{k<k_F}\frac{d^3k}{2\pi} = \frac{2}{(2\pi)^3}V_{\rm FS} \tag{5.52}$$

where

$$V_{\rm FS} = \frac{4\pi}{3}k_F^3 = \left(\frac{4\pi}{3}\right)\left(\frac{2m\epsilon_F}{\hbar^2}\right)^{3/2} \tag{5.53}$$

is the volume of the Fermi surface. The relationship between the density of particles, the Fermi wavevector and the Fermi energy is thus

$$\boxed{\left\langle\frac{\hat{N}}{V}\right\rangle = \frac{1}{3\pi^2}k_F^3 = \frac{1}{3\pi^2}\left(\frac{2m\epsilon_F}{\hbar^2}\right)^{3/2}} \tag{5.54}$$

In an electron gas, where the characteristic density is $N/V \sim 10^{29}m^{-3}$ the characteristic Fermi energy is of order $1eV \sim 10,000K$. In other words, the characteristic energy of an electron is two orders of magnitude larger than would be expected classically. This is a stark and dramatic consequence of the exchange interference between identical particles, and it is one of the great early triumphs of quantum mechanics to have understood this basic piece of physics.

Let us briefly look at finite temperatures. Here, by differentiating the Free energy with respect to volume and chemical potential, we obtain

$$\begin{aligned} P &= -\frac{\partial F}{\partial V} = \frac{-F}{V} = 2k_BT\int_{\mathbf{k}}\ln[1 + e^{-\beta(E_{\mathbf{k}}-\mu)}] \\ N &= -\frac{\partial F}{\partial \mu} = 2\int_{\mathbf{k}} f(E_{\mathbf{k}} - \mu) \end{aligned} \tag{5.55}$$

The second equation *defines* the chemical potential in terms of the particle density at a given temperature. The first equation shows that, apart from a minus sign, the pressure is simply the Free energy density. These two equations can be solved parametrically as a function of chemical potential. At high temperatures the pressure reverts to the ideal gas law $PV = Nk_BT$, but at low temperatures, the pressure is determined by the Fermi energy

$$P = 2\int_{|\mathbf{k}|<k_F}|(\mu - E_{\mathbf{k}})| = \frac{2N}{5V}\epsilon_F \tag{5.56}$$

The final result is obtained by noting that the first term in this expression is $\mu(N/V)$. The first term contains an integral over $d^3k \sim k^2 \to k_F^3/3$, whereas the second term contains an integral over $E_k d^3k \sim k^4 \to k_F^5/5$, so the second term is 3/5 of the first term. Not surprisingly, this quantity is basically the density of fermions times the Fermi energy- a pressure that is hundreds of times larger than the classical pressure in a room temperature electron gas.

Remarks

- At first sight, it might seem very doubtful as to whether the remarkable features of the degenerate Fermi gas would survive once interactions are present. In particular, one would be tempted to wonder whether the Fermi surface would be blurred out by particle-particle interactions. Remarkably, for modest repulsive interactions, the Fermi surface is believed to be stable in dimensions bigger than one. This is because electrons at the Fermi surface have no phase space for scattering. This is the basis of Landau's *Fermi liquid Theory* of interacting Fermions.

- In a remarkable result, due to Luttinger and Ward, the jump in the occupancy at the Fermi wavevector $Z_{\mathbf{k_F}}$ remains finite, although reduced from unity ($Z_{\mathbf{k_F}} < 1$) , in interacting Fermi liquids.

5.3.2 Fluid of Bosons: Bose Einstein Condensation

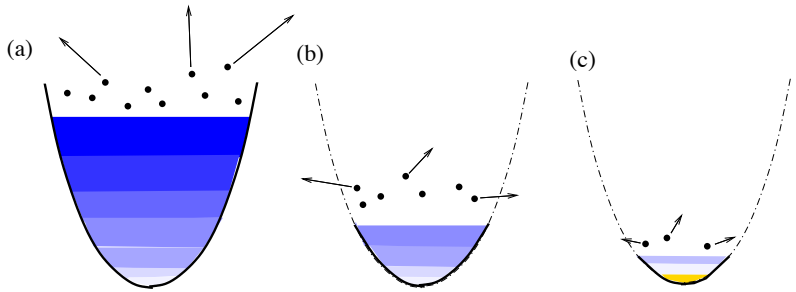

Figure 5.6: Illustrating evaporative cooling in an atom trap. (a) Atoms are held within a magnetic potential. (b) As the height of the potential well is dropped, the most energetic atoms "evaporate" from the well, progressively reducing the temperature. (c) A Bose Einstein condensate, with a finite fraction of the gas in a single momentum state, forms when the temperature drops blow the condensation temperature.

Bose Einstein condensation was predicted in 1924- the outcome of Einstein extending Bose's new calculations on the statistics of a gas of identical bosons. However, it was not until seventy years later- in 1995, that the groups of Cornell and Wieman[5] and independently that of Ketterle[6], succeeded in cooling a low density gas of atoms - initially rubidium and sodium atoms - through the Bose Einstein transition temperature. The closely related phenomenon of superfluidity was first observed in the late 30's by Kapitza. Superfluidity results from a kind of Bose-Einstein condensation, in a dense quantum fluid, where interactions between the particles become important. In the modern context, ultra cold, ultra-dilute gases of alkali atoms are contained inside a magnetic atom trap, in which the Zeeman energy of the atoms, spin-aligned with the magnetic field, confines them

to the region of highest field[7]. Lasers are used to precool a small quantity of atoms inside a magnetic trap using a method known as "Doppler cooling", in which the tiny "blue shift" of the laser light seen by atoms moving towards a laser causes them to selectively absorb photons, which are then re-emitted in a random direction, a process which gradually slows them down, reducing their average temperature. Doppler pre-cooling cools the atoms to about 10-100μK. The second stage involves "Evaporative cooling", a process in which the most energetic atoms are allowed to evaporate out of the well while systematically lowering the height of the well. As the well-height drops, the temperature of the gas plumits down to the nano-Kelvin range required to produce Bose-Einstein condensation (or Fermi liquid formation) in these gases.

To understand the phenomenon of BEC, conside the density of gas of bosons, which at a finite temperature takes almost precisely the same form as for fermions

$$\rho = \int_{\mathbf{k}} \frac{1}{e^{\beta(E_{\mathbf{k}}-\mu)}-1} \tag{5.57}$$

where we have written the expression for spinless bosons, as would be the case for a gas of liquid Helium-4, or ultra-dilute Potassium atoms, for instance. But there is a whole world of physics in the innocent minus sign in the denominator! Whereas for fermions, the chemical potential is positive, the chemical potential for bosons is negative. For a gas at fixed volume , the above expression (5.57) thus defines the chemical potential $\mu(T)$. By changing variables, writing

$$\begin{aligned} x &= \beta E_{\mathbf{k}} = \beta\frac{\hbar^2k^2}{2m}, \qquad \left(\frac{m}{\beta\hbar^2}\right)dx = kdk \\ \frac{d^3k}{(2\pi)^3} &\rightarrow \frac{4\pi k^2dk}{(2\pi)^3} = \frac{1}{\sqrt{2}\pi^2}\left(\frac{m}{\beta\hbar^2}\right)^{3/2}\sqrt{x}dx \end{aligned} \tag{5.58}$$

we can rewrite the Boson density in the form

$$\rho = \frac{2}{\sqrt{\pi}\tilde{\lambda}_T^3}\int_0^\infty dx\,\sqrt{x}\frac{1}{e^{x-\beta\mu}-1} \tag{5.59}$$

where

$$\tilde{\lambda}_T = \left(\frac{2\pi\hbar^2}{mk_BT}\right)^{1/2} \tag{5.60}$$

is a convenient definition of the thermal de Broglie wavelength In order to maintain a fixed density, as one lowers the temperature, the chemical potential $\mu(T)$ must rise. At a certain temperature, the chemical potential becomes zero, $\rho(T,\mu=0) = N/V$ At this temperature,

$$\left(\frac{\tilde{\lambda}_T}{a}\right)^3 = \frac{2}{\sqrt{\pi}}\int_0^\infty dx\,\sqrt{x}\frac{1}{e^x-1} = \zeta(\frac{3}{2}) = 2.61 \tag{5.61}$$

where $a = \rho^{-1/3}$ is the interparticle spacing. The corresponding temperature

$$k_BT_o = 3.31\left(\frac{\hbar^2}{ma^2}\right) \tag{5.62}$$

is the Bose-Einstein condensation temperature.

Below this temperature, the number of Bosons in the $\mathbf{k} = 0$ state becomes macroscopic, i.e.

$$n_{\epsilon=0} = \frac{1}{e^{-\beta\mu} - 1} = N_o(T) \tag{5.63}$$

becomes a finite fraction of the total particle number. Since $N_o(T)$ is macroscopic, it follows that

$$\frac{\mu}{k_B T} = -\frac{1}{N_o(T)} \tag{5.64}$$

is infinitesimally close to zero. For this reason, we must be careful to split off the $\mathbf{k} = 0$ contribution to the particle density, writing

$$N = N_o(T) + \sum_{\mathbf{k}\neq\mathbf{0}} n_{\mathbf{k}} \tag{5.65}$$

and *then* taking the thermodynamic limit of the second term. For the density, this gives

$$\rho = \frac{N}{V} = \rho_0(T) + \int_{\mathbf{k}} \frac{1}{e^{\beta(E_{\mathbf{k}})} - 1} \tag{5.66}$$

The the second term is proportional to $\bar{\lambda}_T{}^{-3} \propto T^{3/2}$. Since the first term vanishes at $T = T_o$, it follows that below the Bose Einstein condensation temperature, the density of bosons in the condensate is thus given by

$$\rho_o(T) = \rho\left[1 - \left(\frac{T}{T_o}\right)^{3/2}\right] \tag{5.67}$$

Remarks

- The Bose Einstein Condensation is an elementary example of a second-order phase transition.
- Bose Einstein condensation is an example of a broken symmetry phase transition. It turns out that the same phenomenon survives in a more robust form, if repulsive interactions between the Bosons are present. In the interacting Bose Einstein Condensate, the field operator $\psi(x)$ for the bosons actually acquires a macroscopic expectation value

$$\langle\psi(x)\rangle = \sqrt{\rho_o}e^{i\phi(x)} \tag{5.68}$$

  In a non-interacting Bose condensate, the phase $\phi(x)$ lacks rigidity, and does not have a well-defined meaning. In an interacting condensate, the phase $\phi(x)$ is uniform, and gradients of the phase result in a *superflow* of particles- a flow of atoms which is completely free from viscosity.

Example 5.1: In a laser-cooled atom trap, atoms are localized in a region of space through the Zeeman energy of interaction between the atomic spin and the external field. As the field changes direction, the "up" and "down" spin atoms adiabatically evolve their orientations to remain parallel with the magnetic field, and the trapping potential of the "up" spin atoms is determined by the magnitude of the Zeeman energy $V(x) = g\mu_B JB(x)$, which has a parabolic form

$$V(x) = \frac{m}{2}\left[\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right]$$

Show that the fraction of bosons condensed in the atom trap is now given by

$$\frac{N_0(T)}{N} = 1 - \left(\frac{T}{T_{BE}}\right)^3.$$

Solution: In the atom trap, one particle states of the atoms are Harmonic oscillator states with energy $E_{lmn} = \hbar(l\omega_x + m\omega_y + n\omega_z)$ (where the constant has been omitted). In this case, the number of particles in the trap is given by

$$N = \sum_{l,m,n} \frac{1}{e^{\beta E_{lmn}} - 1}$$

The summation over the single-particle quantum numbers can be converted to an integral over energy, provided the condensate fraction is split off the sum, so that

$$\sum_{lmn} \frac{1}{e^{\beta E_{lmn}} - 1} = N_0(T) + \int dE\rho(E)\frac{1}{e^{\beta E} - 1},$$

where N_0 is the number of atoms in the condensate and

$$\rho(E) = \sum_{lmn,\ (E_{lmn}\neq 0)} \delta(E - E_{lmn})$$

is the density of states. By converting this sum to an integral we obtain

$$\begin{aligned}
\rho(E) &= \int dl dm dn \delta(E - E_{lmn}) \\
&= \int \frac{dE_x dE_y dE_z}{\hbar\omega_x\hbar\omega_y\hbar\omega_z}\delta(E_x + E_y + E_z - E) \\
&= \frac{1}{(\hbar\bar{\omega})^3}\int_0^E dE_x \int_0^{E_x} dE_y = \frac{E^2}{2(\hbar\bar{\omega})^3}. \qquad (\bar{\omega} = (\omega_x\omega_y\omega_z)^{1/3})
\end{aligned}$$

The quadratic dependence of this function on energy replaces the square-root dependence of the corresponding quantity for free Bosons. The number of particles outside the condensate is proportional to T^3,

$$\int dE\rho(E)\frac{1}{e^{\beta E} - 1} = \frac{T^3}{2(\hbar\bar{\omega})^3}\overbrace{\int dx \frac{x^2}{e^x - 1}}^{2\zeta_3} = N\left(\frac{T}{T_{BE}}\right)^3$$

where $k_B T_{BE} = \hbar\bar{\omega}(N/\zeta_3)^{1/3}$, so that the condensate fraction is now given by

$$\frac{N_0(T)}{N} = 1 - \left(\frac{T}{T_{BE}}\right)^3.$$

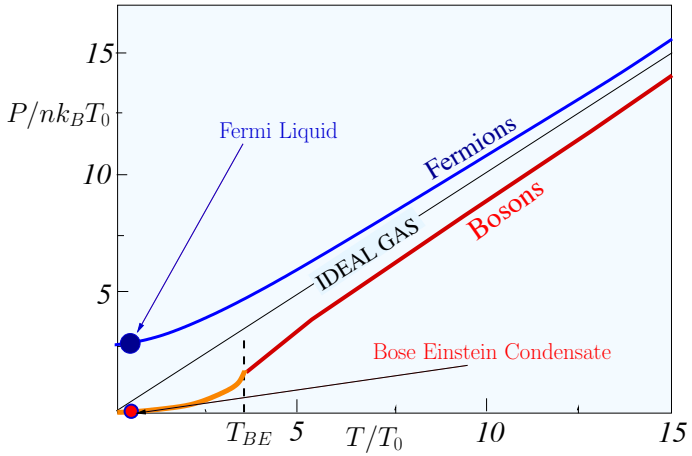

Figure 5.7: Pressure dependence in a Fermi or Bose gas, where temperature is measured in units of $k_BT_0 = \hbar^2/ma^2$ Showing P/nk_B

Example 5.2: Using the results of the previous section, show that the ideal gas law is modified by the interference between identical particles, so that

$$P = nk_BT\mathcal{F}^{\pm}(\mu/k_BT) \tag{5.69}$$

where n is the number density of particles, $\mathcal{F}^{\pm}(z) = g^{\pm}(z)/h^{\pm}(z)$ and

$$\begin{aligned} g^{\pm}(z) &= \pm\int_0^{\infty} dx\,\sqrt{x}\ln[1 \pm e^{-(x-z)}] \\ h^{\pm}(z) &= \int_0^{\infty} dx\,\sqrt{x}\frac{1}{e^{(x-z)} \pm 1} \end{aligned} \tag{5.70}$$

where the upper sign refers to fermions, the bottom to bosons. Sketch the dependence of pressure on temperature for a gas of identical bosons and a gas of identical fermions with the same density.

Solution: Let us begin by deriving an explicit expression for the Free energy of a free gas of fermions, or bosons. We start with

$$F = \mp(2S+1)k_BTV\int_{\mathbf{k}}\ln[1 \pm e^{-\beta(E_{\mathbf{k}}-\mu)}] \tag{5.71}$$

where S is the spin of the particle. Making the change of variables,

$$\begin{aligned} x &= \beta E_{\mathbf{k}} = \beta\frac{\hbar^2k^2}{2m}, \\ \frac{d^3k}{(2\pi)^3} &\rightarrow \frac{2}{\bar{\lambda}_T^3\sqrt{\pi}}\sqrt{x}dx \end{aligned} \tag{5.72}$$

where $\bar{\lambda}_T = \sqrt{2\pi\hbar^2/(mk_BT)}$ is the rescaled Thermal de Broglie wavelength, we obtain

$$F = \mp(2S+1)k_BT\frac{V}{\bar{\lambda}_T^3}\frac{2}{\sqrt{\pi}}\int dx\,\sqrt{x}\ln[1 \pm e^{-(x+\mu\beta)}] \tag{5.73}$$

Taking the derivative with respect to volume, and chemical potential, we obtain the following results for the Pressure and the particle density.

$$\begin{aligned} P &= -\frac{\partial F}{\partial V} = \pm(2S+1)\frac{k_BT}{\bar{\lambda}_T^3}\frac{2}{\sqrt{\pi}}\int dx\,\sqrt{x}\ln[1 \pm e^{-(x-\mu\beta)}] \\ n &= -\frac{\partial F}{V\partial\mu} = \frac{(2S+1)}{\bar{\lambda}_T^3}\frac{2}{\sqrt{\pi}}\int dx\,\sqrt{x}\frac{1}{e^{(x-\mu\beta)} \pm 1} \end{aligned} \tag{5.74}$$

Dividing the pressure by the density, we obtain the quoted result for the ideal gas.

To plot these results, it is convenient to rewrite the temperature and pressure in the form

$$\begin{aligned} T &= T_o[h^{\pm}(\mu\beta)]^{-2/3} \\ \frac{P}{nk_BT_0} &= \frac{g^{\pm}(\mu\beta)}{[h^{\pm}(\mu\beta)]^{5/3}}, \end{aligned} \tag{5.75}$$

where $k_BT_o = \frac{\hbar^2}{ma^2}$, permitting both the pressure and the temperature to be plotted parametrically as a function of $\mu\beta$. Fig 5.7 shows the results of such a plot.

5.4 Exercises

1. (a) Use the Jordan Wigner transformation to show that the one dimensional anisotropic XY model

$$H = -\sum_j[J_1S_x(j)S_x(j+1) + J_2S_y(j)S_y(j+1)] \tag{5.76}$$

can be written as

$$H = -\sum_j[t(d^{\dagger}{}_{j+1}d_j + \text{H.c}) + \Delta(d^{\dagger}{}_{j+1}d^{\dagger}{}_j + \text{H.c})] \tag{5.77}$$

where $t = \frac{1}{4}(J_1+J_2)$ and $\Delta = \frac{1}{4}(J_2-J_1)$.

(b) Calculate the excitation spectrum for this model and sketch your results. Comment specifically on the two cases $J_1 = J_2$ and $J_2 = 0$.

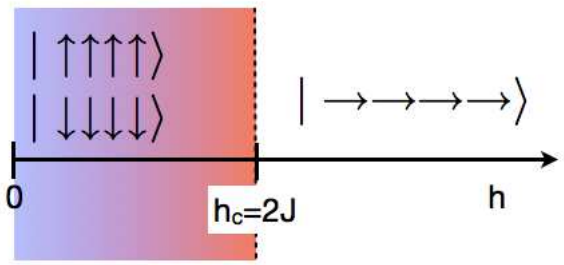

Figure 5.8: Phase diagram of transverse field Ising model. See problem 5.3

2. The 1D transverse field Ising model provides the simplest example of a "quantum phase transition": a phase transition induced by quantum zero point motion (Fig.5.8). This model is written

$$H = -J\sum_j S_z(j)S_z(j+1) - h\sum_j S_x(j),$$

where S_z is the z-component of a spin 1/2, while the the magnetic field h acts in the transverse (x) direction. (For convenience, one can assume periodic boundary conditions, with N_s sites, so that $j = N_s + 1 \equiv j = 0$.) At $h = 0$, the model describes a 1D Ising model, with long-range ferromagnetic order associated with a two fold degenerate ferromagnetic ground state,

$$|\Psi_\uparrow\rangle = |$$

or

$$|\Psi_\downarrow\rangle = |\downarrow_1\rangle|\downarrow_2\rangle\ldots|\downarrow_{N_s}\rangle.$$

A finite transverse field mixes "up" and "down" states, and for infinitely large h, the system has a single ground-state, with the spins all pointing in the x direction,

$$|\Psi_\rightarrow\rangle = \prod_{j=1,N_s}\left(\frac{|\uparrow_j\rangle + |\downarrow_j\rangle}{\sqrt{2}}\right).$$

In other words, there is thus a quantum phase transition- a phase transition driven by quantum fluctuations, between these the doubly degenerate ferromagnet at small h and a singly degenerate state polarized in the x direction at large h.

(a) By rotating the above model so that the magnetic field acts in the +x direction and the Ising interaction acts on the spins in the x direction, the transverse field Ising model can be re-written as

$$H = -J\sum_j S_x(j)S_x(j+1) - h\sum_j S_z(j),$$

(b) Use the Jordan Wigner transformation to show that the fermionized version of this Hamiltonian can be written

$$H = \frac{J}{4}\sum_j (f_j - f^\dagger{}_j)(f_{j+1} + f^\dagger{}_{j+1}) - h\sum_j f^\dagger{}_j f_j. \tag{5.78}$$

(c) Writing $f_j = \frac{1}{\sqrt{N_s}}\sum_k d_k e^{ikR_j}$, where $R_j = aj$, show that H can be rewritten in momentum space as

$$H = \sum_{k\in[0,\pi/a]}\left[\epsilon_k(d^\dagger{}_k d_k - d_{-k}d^\dagger{}_k) + i(\Delta d^\dagger{}_k d^\dagger{}_{-k} - d_{-k}d_k)\right] \tag{5.79}$$

where the sum over $k = \frac{2\pi}{N_s a}(1, 2\ldots N_s/2) \in [0, \frac{\pi}{a}]$ is restricted to half the Brillouin zone, while $\epsilon_k = -\frac{J}{2}\cos ka - h$ and $\Delta_k = \frac{J}{2}\sin ka$.

(d) Using the results of Ex 4.2, show that the spectrum of the excitations are described by "Dirac fermions" with a dispersion

$$E_k = \sqrt{\epsilon_k^2 + \Delta_k^2} = \sqrt{2Jh\sin^2(ka) + (h - J/2)^2}$$

so that gap in the excitation spectrum closes at $h = h_c = 2J$. What is the significance of this field?

3. Consider the non-interacting Hubbard model for next nearest neighbor hopping on a two dimensional lattice

$$H - \mu N = -t\sum_{j,\hat{a}=\hat{x},\hat{y},\sigma}[c^\dagger{}_{j+\hat{a}\sigma}c_{j\sigma} + \text{H.c}] - \mu\sum_{j\sigma} c^\dagger{}_{j\sigma}c_{j\sigma}$$

where $n_{j\sigma} = c^\dagger{}_{j\sigma}c_{j\sigma}$ represents the number of electrons of spin component $\sigma = \pm 1/2$ at site j.

(a) Show that the dispersion of the electrons in the absence of interactions is given by

$$\epsilon(\vec{k}) = -2t(\cos k_x a + \cos k_y a) - \mu$$

where a is the distance between sites, and $\vec{k} = (k_x, k_y)$ is the wavevector.

(b) Derive the relation between the number of electrons per site n_e and the area of the Fermi surface.

(c) Sketch the Fermi surface when

i. $n_e < 1$.

ii. "half filling" where $n_e = 1$

(d) The corresponding interacting Hubbard model, with an interaction term $Un_\uparrow n_\downarrow$ at each site describes a class of material called "Mott insulators", which includes the mother compounds for high temperature superconductors. What feature of the Fermi surface at half-filling makes the non-interacting ground-state unstable to spin density wave formation and the development of a gap around the Fermi surface ?

(e) Derive the dispersion for the case when, in the one-particle Hamiltonian there is an additional next-nearest neighbor hopping matrix element of strength across the diagonal, $-t'$. (Hint: use the Fourier transform of $t(R)$, given by $t(\vec{k}) = \sum_{\vec{R}} t(\vec{R}) e^{-i\vec{k}\cdot\vec{R}}$). How does this affect the dispersion at half filling?

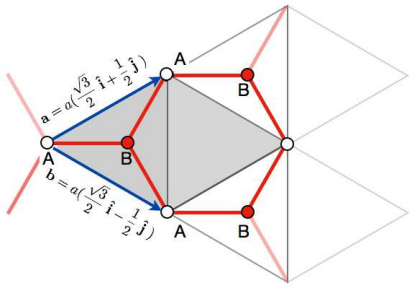

Figure 5.9: Honeycomb structure of graphene. See Problem 5.3

4. Electrons on graphene move on a Honeycomb lattice as shown in Fig. (5.9). The vertices of each unit cell form a triangular lattice of side length a, located at positions $\mathbf{r}_i = m\mathbf{a} + n\mathbf{b}$, where $\mathbf{a} = a\left(\frac{\sqrt{3}}{2}\hat{\mathbf{i}} + \frac{1}{2}\hat{\mathbf{j}}\right)$ and $\mathbf{b} = a\left(\frac{\sqrt{3}}{2}\hat{\mathbf{i}} - \frac{1}{2}\hat{\mathbf{j}}\right)$ are the lattice vectors. There are two atoms per unit cell, labelled "A" and "B". In a simplified model of graphene, electrons can occupy π orbitals at either the A or the B sites, with a tight-binding hopping matrix element $-t$ between neighboring sites.

(a) Construct a tight-binding model for graphene. For simplicity, ignore the spin of the electron. Suppose the creation operator for an electron in the A or B orbital in the "i"th cell is $\psi^\dagger{}_A(\mathbf{r}_i)$, where Show that the tight-binding Hamiltonian can be written in the form

$$H = -t\sum_j \left\{\left[\psi^\dagger{}_B(\mathbf{r}_i) + \psi^\dagger{}_B(\mathbf{r}_i + \mathbf{a}) + \psi^\dagger{}_B(\mathbf{r}_i + \mathbf{b})\right]\psi_A(\mathbf{r}_i) + \text{H.c}\right\} - \mu\sum_i (n_A(i) + n_B(i))$$

(b) By transforming to momentum space, writing $c^\dagger{}_{\mathbf{k}\lambda} = \frac{1}{\sqrt{N_s}}\sum_j \psi^\dagger{}_\lambda(i)e^{i\mathbf{k}\cdot\mathbf{r}_j}$, where $\lambda = A, B$ and N_s is the number of unit cells in the crystal, show that the Hamiltonian can be written

$$H = \sum_{\mathbf{k}} \left(c^\dagger{}_{\mathbf{k}A}, c^\dagger{}_{\mathbf{k}B}\right)\begin{bmatrix} -\mu & \Delta(\mathbf{k}) \\ \Delta^*(\mathbf{k}) & -\mu \end{bmatrix}\begin{pmatrix} c_{\mathbf{k}A} \\ c_{\mathbf{k}B}\end{pmatrix}$$

where

$$\Delta(\mathbf{k}) = -t(1 + e^{i\mathbf{k}\cdot\mathbf{a}} + e^{i\mathbf{k}\cdot\mathbf{b}})$$

with energy eigenstates

$$E(\mathbf{k}) = \pm|\Delta(\mathbf{k})| - \mu.$$

(c) Show that $E(\mathbf{k}) = 0$ at two points in the Brillouin zone where $\mathbf{k}\cdot\mathbf{a} = -\mathbf{k}\cdot\mathbf{b} = \pm\frac{2\pi}{3}$, given by

$$\mathbf{k} = \pm\mathbf{K}$$

where $\mathbf{K} = \frac{4\pi}{3\sqrt{3}a}\hat{\mathbf{i}}$.

(d) By expanding around $\mathbf{k} = \pm\mathbf{K} + \mathbf{p}$, showing that when $\mathbf{p}$ is small, $\Delta_{\mathbf{p}\pm\mathbf{K}} = \tilde{c}(p_x \pm ip_y)$, where $\tilde{c} = \frac{\sqrt{3}}{2}at$ is a "renormalized" speed of light. By defining a spinor for the two cones

$$\psi_{\mathbf{p}+} = \begin{pmatrix} c_{\mathbf{p}+\mathbf{K}A} \\ c_{\mathbf{p}+\mathbf{K}B}\end{pmatrix}, \qquad \psi_{\mathbf{p}-} = \begin{pmatrix} c_{\mathbf{p}-\mathbf{K}B} \\ c_{\mathbf{p}-\mathbf{K}A}\end{pmatrix},$$

show that the Hamiltonian can be written as a Dirac equation

$$H = \sum_{\mathbf{p},l=\pm} \psi^\dagger{}_{\mathbf{p}\lambda}\left(\vec{\sigma}\cdot\mathbf{p} - \mu\underline{1}\right)\psi_{\mathbf{p}\lambda}$$

where $\vec{\sigma}$ is a Pauli pseudo-spin matrix acting in the two-component sublattice space, so that when $\mu = 0$, the excitation spectrum is defined by two Dirac cones with $E(\mathbf{p}) = \pm\tilde{c}p$.

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Chapter 6

Green's Functions

Ultimately, we are interested in more than just free systems. We should like to understand what happens to our system as we dial up the interaction strength from zero, to its full value. We also want to know response of our complex system to external perturbations, such as an electromagnetic field. We have to recognize that we can not, in general expect to diagonalize the problem of interest. We do not even need interactions to make the problem complex: a case in interest is a disordered metal, where we our interest in averaging over typically disordered configurations introduces effects reminiscent of interactions, and can even lead to new kinds of physics, such as electron localization. We need some general way of examinining the change of the system in response to these effects even though we can't diagonalize the Hamiltonian.

In general then, we will be considering problems where we introduce new terms to a non-interaction Hamiltonian, represented by V. The additional term might be due to

- External electromagnetic fields, which modify the Kinetic energy in the Hamiltonian as follows

$$-\frac{\hbar^2}{2m}\nabla^2 \to -\frac{\hbar^2}{2m}\left(\nabla - i\frac{e}{\hbar}\mathbf{A}\right)^2 \tag{6.1}$$

- Interactions between particles.

$$\hat{V} = \frac{1}{2}\int d\mathbf{1}d\mathbf{2}\psi^\dagger(\mathbf{1})\psi^\dagger(\mathbf{2})\psi(\mathbf{2})\psi(\mathbf{1}) \tag{6.2}$$

- A random potential

$$\hat{V} = \int d\mathbf{1}V(\mathbf{1})\rho(\mathbf{1}) \tag{6.3}$$

  where $V(x)$ is a random function of position.

One of the things we would like to do, is to examine what happens when the change in the Hamiltonian to small enough to be considered a perturbation. Even if the term of interest is not small, we can still try to make it small by writing

$$H = H_o + \lambda\hat{V} \tag{6.4}$$

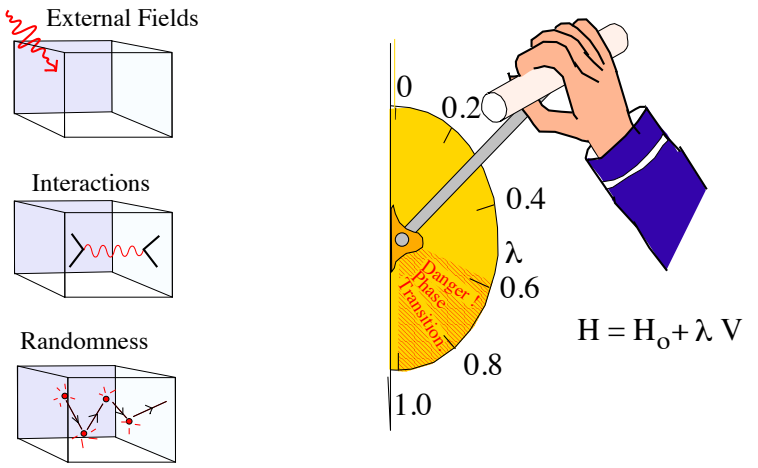


Figure 6.1: "Dialing up the interaction". Motivating the need to be able to treat perturbations to a non-interacting Hamiltonian by dialing up the strength of the perturbation.

This is a useful excercise, for it enables us to consider the effect of adiabatically dialing up the strength of the additional term in the Hamiltonian from zero, to its full value, as illustrated in fig6.1. This is a dangerous procedure, but sometimes it really works. Life is interesting, because in macroscopic systems the perturbation of interest often leads to an instability. This can sometimes occur for arbitrarily small λ. Othertimes, when the instability occurs when the strength of the new term reaches some critical value λ_c. When this happens, the ground-state can change. If the change is a continuous one, then the point where the instability develops is a *Quantum Critical Point*, a point of great interest. Beyond this point, for $\lambda > \lambda_c$, if we are lucky, we can find some new starting $H'_o = H_o + \Delta H$, $\hat{V}' = \hat{V} - \Delta H$. If H'_o is a good description of the ground-state, then we can once again apply this adiabatic procedure, writing,

$$H = H'_o + \lambda'\hat{V}' \tag{6.5}$$

If a phase transition occurs, then H'_o will in all probability have display a spontaneous *broken symmetry*. The region of Hamiltonian space where $H \sim H'_o$ describes a new phase of the system, and H'_o is closely associated with the notion of a "fixed point" Hamiltonian.

All of this discussion motivates us developing a general perturbative approach to many body systems, and this rapidly leads us into the realm of Green's functions and Feynman diagrams. A Green's function describes the elementary correlations and responses of a system. Feynman diagrams are a way of graphically displaying the scattering processes that result from a perturbation.

6.1 Interaction representation

Up until the present, we have known two representations of quantum theory- the Schrödinger representation, where it is the wavefunction that evolves, and the Heisenberg, were the operators evolve and the states are stationary. We are interested in observable quantities more than wavefunctions, and so we aspire to the Heisenberg representation. In practice however, we always want to know what happens if we change the Hamiltonian a little. If we change H_o to $H_o + V$, but we stick to the Heisenberg representation for H_o, then we are now using the "interaction" representation.

Table. 5.1. Representations .

Representation	States	Operators
Schrödinger	Change rapidly $i\frac{\partial}{\partial t}\|\psi_S(t)\rangle = H\|\psi_S(t)\rangle$	O_s- operators constant
Heisenberg	Constant	Evolve $-i\frac{\partial O_H(t)}{\partial t} = [H, O_H(t)]$
Interaction $H = H_o + V$	States change slowly $i\frac{\partial}{\partial t}\|\psi_I(t)\rangle = V_I(t)\|\psi_I(t)\rangle$	Evolve according to H_o $-i\frac{\partial O_I(t)}{\partial t} = [H_o, O_I(t)]$

Let us now examine the interaction representation in greater detail. In the discussion that follows, we simplify the notation by taking taking $\hbar = 1$. We begin by writing the Hamiltonian as two parts $H = H_o + V$. States and operators in this representation are defined as

$$\left.\begin{aligned} |\psi_I(t)\rangle &= e^{iH_o t}|\psi_S(t)\rangle, \\ O_I(t) &= e^{iH_o t}O_S e^{-iH_o t} \end{aligned}\right\} \text{Removes rapid state evolution due to } H_o \tag{6.6}$$

The evolution of the wavefunction is thus

$$\left.\begin{aligned} |\psi_I(t)\rangle &= U(t)|\psi_I(0)\rangle, \\ U(t) &= e^{iH_o t}e^{-iHt} \end{aligned}\right\} \tag{6.7}$$

or more generally,

$$|\psi_I(t)\rangle = S(t,t')|\psi_I(t')\rangle,$$

$$S(t) = U(t)U^\dagger(t') \tag{6.8}$$

The time evolution of $U(t)$ can be derived as follows

$$\begin{aligned} i\frac{\partial U}{\partial t} &= i\left(\frac{\partial e^{iH_o t}}{\partial t}\right)e^{-iHt} + ie^{iH_o t}\left(\frac{\partial e^{-iHt}}{\partial t}\right) \\ &= e^{iH_o t}(-H_o + H)e^{-iHt} \\ &= [e^{iH_o t}Ve^{-iH_o t}]U(t) \\ &= V_I(t)U(t) \end{aligned} \tag{6.9}$$

so that

$$i\frac{\partial S(t_2,t_1)}{\partial t_1} = V(t_2)S(t_2,t_1) \tag{6.10}$$

where from now on, all operators are implicitly assumed to be in the interaction representation.

Now we should like to exponentiate this time-evolution equation, but unfortunately, the operator $V(t)$ is not constant, and furthermore, $V(t)$ at one time, does not commute with $V(t')$ at another time. To overcome this difficulty, Schwinger invented a device called the "time-ordering operator".

Time ordering operator Suppose $\{O_1(t_1), O_2(t_2)\ldots O_N(t_N)\}$ is a set of operators at different times $\{t_1, t_2 \ldots t_N\}$. If P is the permutation that orders the times, so that $t_{P_1} > t_{P_2} \ldots t_{P_N}$, then if the operators are entirely bosonic, containing an even number of fermionic operators,the time ordering operator is defined as

$$T[O_1(t_1)O_2(t_2)\ldots O_N(t_N)] = O_{P_1}(t_{P_1})O_{P_2}(t_{P_2})\ldots O_{P_N}(t_{P_N}) \tag{6.11}$$

For later use, we note that if the operator set contains fermionic operators, composed of an odd number of fermionic operators, then

$$T[F_1(t_1)F_2(t_2)\ldots F_N(t_N)] = (-1)^P F_{P_1}(t_{P_1})F_{P_2}(t_{P_2})\ldots F_{P_N}(t_{P_N}) \tag{6.12}$$

where P is the number of pairwise permutations of fermions involved in the time ordering process.

Suppose we divide the time interval $[t_1, t_2]$, where $t_2 > t_1$ into N identical segments of period $\Delta t = (t_2 - t_1)/N$, where the time at the midpoint of the *nth* segment is $\tau_n = t_1 + (n - \frac{1}{2})\Delta t$. The S-matrix can be written as a product of S-matrices over each intermediate time segment, as follows:

$$S(t_2,t_1) = S(t_2, \tau_N - \tfrac{\Delta t}{2})S(\tau_{N-1} + \tfrac{\Delta t}{2}, \tau_{N-1} - \tfrac{\Delta t}{2})\ldots S(\tau_1 + \tfrac{\Delta t}{2}, t_1) \tag{6.13}$$

Provided N is large, then over the short time interval Δt, we can approximate

$$S(\tau + \tfrac{\Delta t}{2}, \tau - \tfrac{\Delta t}{2}) = e^{-iV(\tau)\Delta t} + O(1/N^2) \tag{6.14}$$

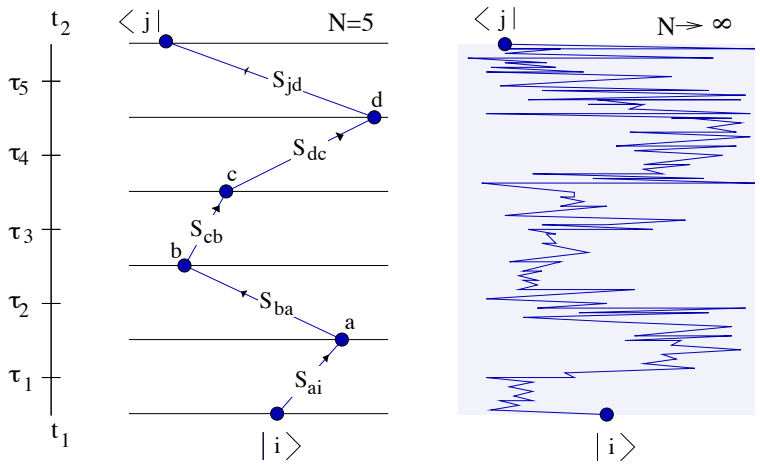


Figure 6.2: Each contribution to the time-ordered exponential corresponds to the amplitude to follow a particular path in state space. The S-matrix is given by the limit of the process where the number of time segments is sent to infinity.

so that we can write

$$S(t_2,t_1) = e^{-iV(\tau_N)\Delta t}e^{-iV(\tau_{N-1})\Delta t}\ldots e^{-iV(\tau_1)\Delta t} + O(1/N) \tag{6.15}$$

Using the time-ordering operator, this can be written

$$S(t_2,t_1) = T[\prod_{j=1}^{N} e^{-iV(\tau_j)\Delta t}] + O(1/N) \tag{6.16}$$

The beauty of the time-ordering operator, is that even though $A(t_1)$ and $A(t')$ don't commute, we can treat them as commuting operators so long as we always time-order them. This means that we can write

$$T[e^{A(t_1)}e^{A(t_2)}] = T[e^{A(t_1)+A(t_2)}] \tag{6.17}$$

because in each time-ordered term in the Taylor expansion, we never have to commute operators, so the algebra is the same as for regular complex numbers. With this trick, we can write,

$$S(t_2,t_1) = Lim_{N\to\infty}T[e^{-i\sum_j V(\tau_j)\Delta t}] \tag{6.18}$$

The limiting value of this time-ordered exponential is written as

$$S(t_2,t_1) = T\Big[\exp\Big\{-i\int_{t_1}^{t_2} V(t)dt\Big\}\Big], \qquad \textbf{Time-ordered exponential} \tag{6.19}$$

This is the famous time-ordered exponential of the interaction representation.

Remarks

- The time-ordered exponential is intimately related to Feynman's notion of the path integral. The time-evolution operator $S(\tau_j + \Delta\tau/2, \tau_j - \Delta\tau/2) = S_{fr}(\tau_j)$ across each segment of time is a matrix that takes one from state r to state f. The total time evolution operator is just a matrix product over each intermediate time segment. Thus the amplitude to go from state i at time t_1 to state f at time t_2 is given by

$$S_{fi}(t_2,t_1) = \sum_{\text{path}=\{p_1,\ldots p_{N_1}\}} S_{f,p_{N-1}}(\tau_N)\ldots S_{p_2p_1}(\tau_2)S_{p_1i}(\tau_1) \tag{6.20}$$

  Each term in this sum is the amplitude to go along the path of states

$$\text{path } i \;\to\; f: \; i \to p_1 \to p_2 \to \ldots p_{N-1} \to f. \tag{6.21}$$

  The limit where the number of segments goes to infinity is a path integral.

- One can formally expand the time-ordered exponential as a power series, writing,

$$S(t_2,t_1) = \sum_{n=0,\infty}\frac{(-i)^n}{n!}\int_{t_1}^{t_2} d\tau_1\ldots d\tau_n T[V(\tau_1)\ldots V(\tau_n)] \tag{6.22}$$

  The *nth* term in this expansion can be simply interpreted as the amplitude to go from the initial, to the final state, scattering n times off the perturbation V. This form of the S-matrix is very useful in making a perturbation expansion. By explicitly time-ordering the $n-th$ term, one obtains $n!$ identical terms, so that

$$S(t_2,t_1) = \sum_{n=0,\infty}(-i)^n\int_{t_1,\ \{\tau_n>\tau_{n-1}\cdots>\tau_1\}}^{t_2} d\tau_1\ldots d\tau_n V(\tau_n)\ldots V(\tau_1) \tag{6.23}$$

  This form for the S-matrix is obtained by iterating the equation of motion,

$$S(t_2,t_1) = 1 - i\int_{t_1}^{t_2} d\tau V(\tau)S(\tau,t_1) \tag{6.24}$$

  which provides an alternative derivation of the time-ordered exponential.

6.1.1 Driven Harmonic Oscillator

To illustrate the concept of the time-ordered exponential, we shall show how it is possible to evaluate the S-matrix for a driven harmonic oscillator, where $H = H_o + V(t)$,

$$\left.\begin{array}{rcl} H_o & = & \omega(b^\dagger b + \frac{1}{2}) \\ V(t) & = & \bar{z}(t)b + b^\dagger z(t) \end{array}\right\} \tag{6.25}$$

Here the forcing terms are written in their most general form. $z(t)$ and $\bar{z}(t)$ are forces which "create" and "annihilate" quanta respectively. A conventional force in the Hamiltonian, $H = H_o - f(t)\hat{x}$ gives rise to a particular case, where $\bar{z}(t) = z(t) = (1/2m\omega)^{\frac{1}{2}} f(t)$. We shall show that if the forcing terms are zero in the distant past and distant future and the system is initially in the ground-state, the amplitude to stay in this state is

$$\boxed{\langle 0|Te^{-i\int_{-\infty}^{\infty} dt[\bar{z}(t)b(t)+b^\dagger(t)z(t)]}|0\rangle = \exp\left[-i\int_{-\infty}^{\infty} dtdt'\bar{z}(t)G(t-t')z(t')\right].} \tag{6.26}$$

where $G(t-t') = -i\theta(t-t')e^{-i\omega(t-t')}$ is our first example of a one particle "Green's function". The importance of this result, is that we have a precise algebraic result for the response of the ground-state to an arbitrary force term. Once we know the response to an arbitrary force, we can, as we shall see, deduce the n-th ordered moments, or correlation functions of the Bose fields.

Remarks:

- The time-ordered exponential is an example of a "functional": a quantity which is a function of a function (in this case, $z(t)$ and $\bar{z}(t)$). With this result we can examine how the ground-state responds to an arbitrary external force. The quantity $G(t-t')$ which determines the response of the ground-state to the forces, $z(t)$ and $\bar{z}(t)$, is called the "one particle Green's function", defined by the relation

$$G(t-t') = -i\langle 0|Tb(t)b^\dagger(t')|0\rangle. \tag{6.27}$$

  We may confirm this relation by expanding both sides of (6.26) to first order in $\bar{z}$ and z. The left hand side gives

$$1 + (-i)^2\int dtdt'\bar{z}(t)\langle 0|Tb(t)b^\dagger(t')|0\rangle.z(t') + O(\bar{z}^2, z^2) \tag{6.28}$$

  whereas the right-hand side gives

$$1 - i\int dtdt'\bar{z}(t)G(t-t')z(t') + O(\bar{z}^2, z^2) \tag{6.29}$$

  By comparing the coefficients, we are able to confirm the above relation.

- By expanding the time-ordered exponential as a power-series in z and $\bar{z}$, we find that the n-th order term is

$$\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}\prod_{r=1,n} dt_r dt'_r \bar{z}(t_r)z(t'_r) \times \text{ coeff} \tag{6.30}$$

  where

$$\text{coeff} = G(1,\ldots n;1'\ldots n') = (-i)^n\langle 0|Tb(1)\ldots b(n)b^\dagger(n')\ldots b^\dagger(1')|0\rangle \tag{6.31}$$

  is called the n-particle Green's function. Here we have used the conventient notation $r \equiv t_r$, $r' \equiv t'_r$. By expanding the right-hand-side, we find that the corresponding coefficient of z and $\bar{z}$ is given by the sum over all possible ways of connecting initial times $\{r'\}$ with final times $\{r\}$ by a single-particle Green's function,

$$G(1,\ldots n;1'\ldots n') = \sum_P \prod_r G(r - P'_r), \tag{6.32}$$

  a result known as Wick's theorem. It is a remarkable property of non-interacting systems, that the n-particle Green's functions are determined entirely in terms of the one-particle Green functions. In (6.32) each destruction event at time $t_r \equiv r$ is paired up with a corresponding creation event at time $t'_{P_r} \equiv P'_r$. The connection between these two events is often called a "contraction", denoted as follows

$$(-i)^n\langle\phi|T\ldots b(r)\ldots b^\dagger(P'_r)\ldots|\phi\rangle \quad = G(r-P'_r)\times(-i)^{n-1}\langle 0|T\ldots|0\rangle \tag{6.33}$$

  Notice that since particles are conserved, we can only contract a creation operator with a destruction operator. According to Wick's theorem, the expansion of the n-particle Green function in (6.31) is carried out as a sum over all possible contractions, denoted as follows

$$G(1\ldots n') = \sum_P G(1-P'_1)G(2-P'_2)\ldots G(r-P'_r)\ldots$$

$$= \sum_P (-i)^n\langle\phi|Tb(1)b(2)\ldots b(r)\ldots b^\dagger(P'_r)\ldots b^\dagger(P'_1)\ldots b^\dagger(P'_2)\ldots|\phi\rangle \tag{6.34}$$

  Physically, this result follows from the identical nature of the bosonic quanta or particles. When we take the n particles out at times $t_1\ldots t_n$, there is no way to know in which order we are taking them out. The net amplitude is the sum of all possible ways of taking out the particles- This is the meaning of the sum over permutations P.

- This result can be generalized to an arbitrary number of oscillators by replacing $(z,\ \bar{z}) \to (z_r, \bar{z}_r)$, whereupon

$$\begin{aligned} &\langle\ 0|T\exp\left[-i\int_{-\infty}^{\infty} dt[\bar{z}_r(t)b_r(t) + b_r{}^{\dagger}(t)z_r(t)]\right]|0\rangle \\ &= \exp\left[-i\int_{-\infty}^{\infty} dtdt'\bar{z}_r(t)G_{rs}(t-t')z_s(t')\right] \end{aligned} \tag{6.35}$$

  where now, $G_{rs}(t-t') = -i\langle 0|Tb_r(t)b^{\dagger}{}_s(t')|0\rangle = -i\delta_{rs}\theta(t-t')e^{-i\omega_r(t-t')}$, and summation over repeated indices is implied. This provides the general basis for Wick's theorem.

- The concept of a generating functional can also be generalized to Fermions, with the proviso that now we must use replace $(z, \bar{z})$ by anticommuting numbers $(\eta, \bar{\eta})$.

Proof: To demonstrate this result, we need to evaluate the time ordered exponential

$$\langle\ \ 0\ \ |T\exp\left[-i\int_{-t_1}^{t_2} dt[\bar{z}(t)b(t) + b^{\dagger}(t)z(t)]\right]|0\rangle \tag{6.36}$$

where $b(t) = be^{i\omega t}$ and $b^{\dagger}(t) = b^{\dagger}e^{i\omega t}$. To evaluate this integral, we divide up the interval $t \in (t_1, t_2)$ into N segments, $t \in (\tau_j - \Delta\tau/2, \tau_j + \Delta\tau_j)$ of width $\Delta\tau = (t_2 - t_1)/N$ and write down the discretized time-ordered exponential as

$$S_N = e^{A_N - A^{\dagger}{}_N} \times \ldots e^{A_r - A^{\dagger}{}_r} \times \ldots e^{A_1 - A^{\dagger}{}_1} \tag{6.37}$$

where we have used the short-hand notation,

$$\begin{aligned} A_r &= -i\bar{z}(\tau_r)b(\tau_r)\Delta\tau, \\ A^{\dagger}{}_r &= ib^{\dagger}(\tau_r)z(\tau_r)\Delta\tau \end{aligned} \tag{6.38}$$

To evaluate the ground-state expectation of this exponential, we need to "normal" order the exponential, bringing the terms involving annihilation operators e^{A_r} to the right-hand side of the expression. To do this , we use the result

$$e^{\alpha+\beta} = e^{\beta}e^{\alpha}e^{[\alpha,\beta]/2} \tag{6.39}$$

to separate $e^{A_r - A^{\dagger}{}_r} \to e^{-A^{\dagger}{}_r}e^{A_r}e^{-[A_r, A^{\dagger}{}_r]/2}$, and the related result

$$e^{\alpha}e^{\beta} = e^{\beta}e^{\alpha}e^{[\alpha,\beta]} \tag{6.40}$$

to commute the e^{A_r} to the right, past terms of the form $e^{-A^{\dagger}{}_s}$, $e^{A_r}e^{-A^{\dagger}{}_s} = e^{-A^{\dagger}{}_s}e^{A_r}e^{-[A_r, A^{\dagger}{}_s]}$. These expressions hold if $[\alpha,\beta]$ commutes with α and β [1] . We observe that in our case,

$$[A_r, A^{\dagger}{}_s] = \Delta\tau^2\bar{z}(\tau_r)z(\tau_s)e^{-i\omega(\tau_r - \tau_s)} \tag{6.41}$$

[1]To prove this result consider $\hat{f}(x) = e^{x\hat{\alpha}}e^{\hat{\beta}}e^{-x\hat{\alpha}}$. First, $df/dx = e^{x\hat{\alpha}}[\hat{\alpha}, e^{\hat{\beta}}]e^{-x\hat{\alpha}}$. By expanding $e^{\hat{\beta}}$ as a power series, one can confirm that $[\hat{\alpha}, e^{\hat{\beta}}] = [\hat{\alpha}, \hat{\beta}]e^{\hat{\beta}}$, provided $[\hat{\alpha}, \hat{\beta}]$ commutes with $\hat{\beta}$. It follows that $df/dx = e^{x\hat{\alpha}}[\hat{\alpha}, \hat{\beta}]e^{\hat{\beta}}e^{-x\hat{\alpha}}$. Now provided $[\hat{\alpha}, \hat{\beta}]$ also commutes with $\hat{\alpha}$, then $e^{x\hat{\alpha}}[\hat{\alpha}, \hat{\beta}] = [\hat{\alpha}, \hat{\beta}]e^{x\hat{\alpha}}$, so it follows that $df/dx = [\hat{\alpha}, \hat{\beta}]f(x)$. Since $[\hat{\alpha}, \hat{\beta}]$ commutes with with $f[x]$, the solution to this equation is simply $f[x] = e^{x[\hat{\alpha}, \hat{\beta}]}f[0] = e^{x[\hat{\alpha}, \hat{\beta}]}e^{\hat{\beta}}$. Setting $x = 1$, it follows that $f(1) = e^{\hat{\alpha}}e^{\hat{\beta}}e^{-\hat{\alpha}} = e^{[\hat{\alpha}, \hat{\beta}]}e^{\hat{\beta}}$, from which $e^{\alpha}e^{\beta} = e^{\beta}e^{\alpha}e^{[\alpha,\beta]}$.

is a c-number, so we can use the above theorem. We first normal order each term in the product, writing $e^{A_r - A^{\dagger}{}_r} = e^{-A^{\dagger}{}_r}e^{A_r}e^{-[A_r, A^{\dagger}{}_r]/2}$ so that

$$S_N = e^{-A^{\dagger}{}_N}e^{A_N}\ldots e^{-A^{\dagger}{}_1}e^{A_1}e^{-\sum_r[A_r, A^{\dagger}{}_r]/2} \tag{6.42}$$

Now we move the general term e^{A_r} to the right-hand side, picking up the residual commutators along the way to obtain

$$S_N = \overbrace{e^{-\sum_r A^{\dagger}{}_r}e^{\sum_r A_r}}^{:S_N:} \exp[-\sum_{r\geq s}[A_r, A^{\dagger}{}_s](1 - \frac{1}{2}\delta_{rs})], \tag{6.43}$$

where the δ_{rs} term is present because by Eq. (6.42), we get half a commutator when $r = s$. The vacuum expectation value of the first term is unity, so that

$$\begin{aligned} S(t_2, t_1) &= \lim_{\Delta\tau\to 0}\exp\Big[-\sum_{s\leq r}\Delta\tau^2\bar{z}(\tau_r)z(\tau_s)e^{-i\omega(\tau_r - \tau_s)}(1 - \frac{1}{2}\delta_{rs})\Big] \\ &= \exp\Big[-\int_{t_1}^{t_2} d\tau d\tau'\bar{z}(\tau)\theta(\tau - \tau')e^{-i\omega(\tau - \tau')}z(\tau')\Big], \end{aligned} \tag{6.44}$$

where the δ_{rs} term contributes a term of order $\Delta\tau\int_{t_1}^{t_2} d\tau|z(\tau)|^2\ O(\Delta\tau)$ to the exponent that vanishes in the limit $\Delta\tau \to 0$. So placing $G(t-t') = -i\theta(\tau - \tau')e^{-i\omega(\tau-\tau')}$,

$$S(t_2, t_1) = \exp\Big[-i\int_{t_1}^{t_2} d\tau d\tau'\bar{z}(\tau)G(t-t')z(\tau')\Big] \tag{6.45}$$

Finally, taking the limits of the integral to infinity, we obtain the quoted result.

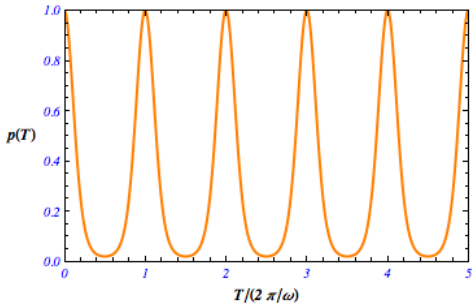


Figure 6.3: Probability $p(T)$ for an oscillator to remain in its ground-state after exposure to an electric field for time T, illustrated for the case $V/\hbar\omega = 1$.

Example 6.1: A charged particle of charge q, mass m is in the ground-state of a harmonic potential of characteristic frequency ω. Show that after exposure to an electric field E for a time T, the probability it remains in the ground-state is given by

$$p = \exp[-4g^2 \sin^2(\omega T/2)] \tag{6.46}$$

where the coupling constant

$$g^2 = \frac{V_{spring}}{\hbar\omega} \tag{6.47}$$

is the ratio between the potential energy $V_{spring} = q^2E^2/(2m\omega^2)$ stored in a classical spring stretched by a force qE and the quantum of energy $\hbar\omega$.

Solution: The probability $p = |S(T,0)|^2$, to remain in the ground-state is the square of the amplitude

$$S(T,0) = \langle\phi|Te^{-\frac{i}{\hbar}\int_0^T V(t)dt}|\phi\rangle. \tag{6.48}$$

Notice, that since we explicitly re-introduced $\hbar \neq 1$, we must now use

$$\frac{V(t)}{\hbar} = -\frac{qE(t)}{\hbar}x(t) \tag{6.49}$$

in the time-ordered exponential, where $E(t)$ is the electric field. Writing $x = \sqrt{\frac{\hbar}{2m\omega}}(b + b^\dagger)$, we can recast V in terms of boson creation and annihilation operators as $V(t)/\hbar = \bar{z}(t)b(t) + b^\dagger(t)z(t)$, where,

$$z(t) = \bar{z}(t) = -\frac{1}{\hbar}\sqrt{\frac{\hbar}{2m\omega}}qE(t) = -\sqrt{\frac{V\omega}{\hbar}}\theta(t). \tag{6.50}$$

Here $V = \frac{q^2E^2}{2m\omega^2}$ is the potential energy of the spring in a constant field E Using the relationship derived in (6.45), we deduce that

$$S(T,0) = e^{-iA}$$

where the phase term

$$A = \int_0^T dt_1 dt_2 \bar{z}(t_1)G(t_1 - t_2)z(t_2)$$

and $G(t) = -ie^{-i\omega t}\theta(t)$ is the Green function. Carrying out the integral, we obtain

$$\begin{aligned} A &= -i\frac{V\omega}{\hbar}\int_0^T dt\int_0^t dt' e^{-i\omega(t-t')} = -\frac{VT}{\hbar} + \frac{2V}{\hbar\omega}e^{-i\omega T/2}\sin\frac{\omega T}{2} \\ &= -\frac{VT}{\hbar}\left[1 - \frac{\sin(\omega T)}{\omega T}\right] - i\frac{2V}{\hbar\omega}\sin^2\left(\frac{\omega T}{2}\right). \end{aligned} \tag{6.51}$$

The real part of A contains a term that grows linearly in time, $ReA \sim -VT/\hbar$ giving rise to uniform growth in the phase of $S(T) \sim e^{iVT/\hbar}|S(T,0)|$ that we recognize as a consequence of the shift in the ground-state energy of the oscillator $E_g \to \frac{\hbar\omega}{2} - V$ in the applied field. The imaginary part determines the probability to remain in the ground-state, which is given by

$$p = |S(T,0)|^2 = e^{2Im[A]} = \exp\left(-\frac{4V}{\hbar\omega}\sin^2\frac{\omega T}{2}\right).$$

demonstrating the oscillatory amplitude to remain in the ground-state (Fig. 6.3).

6.2 Green's Functions

Green's functions are the elementary response functions of a many body system. The one particle Green's function is defined as

$$G_{\lambda\lambda'}(t - t') = -i\langle\phi|T\psi_\lambda(t)\psi^\dagger{}_{\lambda'}(t')|\phi\rangle \tag{6.52}$$

where $|\phi\rangle$ is the many body ground-state, $\psi_\lambda(t)$ is the field in the Heisenberg representation and

$$T\psi_\lambda(t)\psi^\dagger{}_{\lambda'}(t') = \begin{cases} \psi_\lambda(t)\psi^\dagger{}_{\lambda'}(t') & (t > t') \\ \pm\psi^\dagger{}_{\lambda'}(t')\psi_\lambda(t) & (t < t') \end{cases} \qquad \pm \begin{cases} \text{Bosons} \\ \text{Fermions} \end{cases} \tag{6.53}$$

defines the time-ordering for fermions and bosons. Diagramatically, this quantity is represented as follows

$$G_{\lambda\lambda'}(t - t') = \quad \lambda,t \longleftarrow \lambda',t' \tag{6.54}$$

Quite often, we shall be dealing with translationally invariant systems, where λ denotes the momentum and spin of the particle $\lambda \equiv \mathbf{p}\sigma$. If spin is a good quantum number, (no magnetic field, no spin-orbit interactions), then

$$G_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}(t - t') = \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}G(\mathbf{k}, t - t') \tag{6.55}$$

is diagonal, (where in the continuum limit, $\delta_{\mathbf{k}\mathbf{k}'} \to (2\pi)^D\delta^{(D)}(\mathbf{k} - \mathbf{k}')$). In this case, we denote

$$G(\mathbf{k}, t - t') = -i\langle\phi|T\psi_{\mathbf{k}\sigma}(t)\psi^\dagger{}_{\mathbf{k}\sigma}(t')|\phi\rangle = \quad t \xleftarrow{\mathbf{k}} t' \tag{6.56}$$

We can also define Green's function in co-ordinate space,

$$G(\mathbf{x} - \mathbf{x}', t) = -i\langle\phi|T\psi_\sigma(\mathbf{x}, t)\psi^\dagger{}_\sigma(\mathbf{x}', t')|\phi\rangle \tag{6.57}$$

which we denote diagramatically, by

$$G(\mathbf{x} - \mathbf{x}', t) = \text{(x,t)} \longleftarrow \text{(x',t')} \tag{6.58}$$

By writing $\psi_\sigma(\mathbf{x}, t) = \int_{\mathbf{k}}\psi_{\mathbf{k}\sigma}e^{i(\mathbf{k}\cdot\mathbf{x})}$, we see that the co-ordinate-space Green's function is just the Fourier transform of the momentum-space Green's function:

$$\begin{aligned} G(\mathbf{x} - \mathbf{x}', t) &= \int_{\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}\cdot\mathbf{x} - \mathbf{k}'\cdot\mathbf{x}')}\overbrace{-i\langle\phi|T\psi_{\mathbf{k}\sigma}(t)\psi^\dagger{}_{\mathbf{k}'\sigma}(0)|\phi\rangle}^{\delta_{\mathbf{k}\mathbf{k}'}G(\mathbf{k},t-t')} \\ &= \int\frac{d^3k}{(2\pi)^3}G(\mathbf{k}, t)e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \end{aligned} \tag{6.59}$$

It is also often convenient to Fourier transform in time, so that

$$G(\mathbf{k}, t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}G(\mathbf{k}, \omega)e^{-i\omega t} \tag{6.60}$$

The quantity

$$G(\mathbf{k},\omega) = \int_{-\infty}^{\infty} dt G(\mathbf{k},t)e^{i\omega t} = \quad \mathbf{k},\omega \quad \text{(6.61)}$$

is known as the propagator. We can then relate the Green's function in co-ordinate space to its propagator, as follows

$$-i\langle\phi|T\psi_\sigma(\mathbf{x},t)\psi^\dagger{}_\sigma(\mathbf{x}',t')|\phi\rangle = \int \frac{d^3kd\omega}{(2\pi)^4} G(\mathbf{k},\omega)e^{i[(\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')-\omega(t-t')]} \quad \text{(6.62)}$$

6.2.1 Green's function for free Fermions

As a first example, let us calculate the Green's function of a degenerate Fermi liquid of non-interacting Fermions in its ground-state. We shall take the heat-bath into account, using a Heisenberg representation where the heat-bath contribution to the energy is subtracted away, so that

$$H = \hat{H}_o - \mu N = \sum_\sigma \epsilon_{\mathbf{k}} c^\dagger{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}. \quad \text{(6.63)}$$

is the Hamiltonian used in the Heisenberg representation and $\epsilon_{\mathbf{k}} = \frac{\hbar^2k^2}{2m} - \mu$. The ground-state for a fluid of fermions is given by

$$|\phi\rangle = \prod_{\sigma|\mathbf{k}|<k_f} c^\dagger{}_{\mathbf{k}\sigma}|0\rangle \quad \text{(6.64)}$$

In the Heisenberg representation, $c^\dagger{}_{\mathbf{k}\sigma}(t) = e^{i\epsilon_{\mathbf{k}}t}c^\dagger{}_{\mathbf{k}\sigma}$, $c_{\mathbf{k}\sigma}(t) = e^{-i\epsilon_{\mathbf{k}}t}c_{\mathbf{k}\sigma}$. For forward time propagation, it is only possible to add a fermion above the Fermi energy, and

$$\begin{aligned}\langle\phi|c_{\mathbf{k}\sigma}(t)c^\dagger{}_{\mathbf{k}'\sigma'}(t')|\phi\rangle &= \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}e^{-i\epsilon_{\mathbf{k}}(t-t')}\langle\phi|c_{\mathbf{k}\sigma}c^\dagger{}_{\mathbf{k}\sigma}|\phi\rangle \\ &= \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}(1-n_{\mathbf{k}})e^{-i\epsilon_{\mathbf{k}}(t-t')}\end{aligned} \quad \text{(6.65)}$$

where $n_{\mathbf{k}} = \theta(|k_F| - |\mathbf{k}|)$. For backward time propagators, it is only possible to destroy a fermion, creating a hole, below the Fermi energy

$$\langle\phi|c^\dagger{}_{\mathbf{k}'\sigma'}(t')c_{\mathbf{k}\sigma}(t)|\phi\rangle = \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}n_{\mathbf{k}}e^{-i\epsilon_{\mathbf{k}}(t-t')} \quad \text{(6.66)}$$

so that

$$G(\mathbf{k},t) = -i[(1-n_{\mathbf{k}})\theta(t) - n_{\mathbf{k}}\theta(-t)]e^{-i\epsilon_{\mathbf{k}}t} \quad \text{(6.67)}$$

can be expanded as

$$G(\mathbf{k},t) = \begin{cases} -i\theta_{|\mathbf{k}|-|\mathbf{k}_F|}e^{-i\epsilon_{\mathbf{k}}t} & (t>0) \quad \text{“electrons”} \\ i\theta_{|\mathbf{k}_F|-|\mathbf{k}|}e^{-i\epsilon_{\mathbf{k}}t} & (t<0) \quad \text{“holes” : electrons moving backwards in time} \end{cases} \quad \text{(6.68)}$$

This unification of hole and electron excitations in a single function is one of the great utilities of the time-ordered Green's function. [2]

Next, let us calculate the Fourier transform of the Green's function. This is given by

$$\begin{aligned}G(\mathbf{k},\omega) &= -i\int_{-\infty}^{\infty} dt e^{i(\omega-\epsilon_{\mathbf{k}})t} \quad \overbrace{e^{-|t|\delta}}^{\text{cnvgnce factor}} \quad \Big[\theta_{k-k_F}\theta(t) - \theta_{k_F-k}\theta(-t)\Big] \\ &= -i\Big[\frac{\theta_{k-k_F}}{\delta - i(\omega-\epsilon_{\mathbf{k}})} - \frac{\theta_{k_F-k}}{\delta + i(\omega-\epsilon_{\mathbf{k}})}\Big] = \frac{1}{\omega - \epsilon_{\mathbf{k}} + i\delta_{\mathbf{k}}}\end{aligned} \quad \text{(6.69)}$$

where $\delta_{\mathbf{k}} = \text{sign}(\text{k} - \text{k}_\text{F})$. The free fermion propagator is then

$$G(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} + i\delta_{\mathbf{k}}} = \quad \mathbf{k},\omega \quad \text{(6.70)}$$

The Green's function contains both static, and dynamic information about the motion of particles in the many-body system. For example, we can use it to calculate the density of particles in a Fermi gas

$$\begin{aligned}\langle\hat{\rho}(x)\rangle &= \sum_\sigma \langle\psi^\dagger{}_\sigma\psi_\sigma\rangle = -\sum_\sigma \langle\phi|T\psi_\sigma(x,0^-)\psi^\dagger{}_\sigma(x,0)|\phi\rangle \\ &= -i(2S+1)G(\mathbf{x},0^-)|_{\mathbf{x}=0}\end{aligned} \quad \text{(6.71)}$$

where S is the spin of the fermion. We can also use it to calculate the Kinetic energy density, which is given as follows

$$\begin{aligned}\langle\hat{T}(x)\rangle &= -\frac{\hbar^2}{2m}\sum_\sigma \langle\psi^\dagger{}_\sigma(x)\nabla_x^2\psi_\sigma(x)\rangle = \frac{\hbar^2\nabla_x^2}{2m}\sum_\sigma \langle\phi|T\psi_\sigma(x,0^-)\psi^\dagger{}_\sigma(\vec{x}',0)|\phi\rangle\Big|_{\mathbf{x}-\mathbf{x}'=\mathbf{0}} \\ &= i(2S+1)\,\frac{\hbar^2\nabla^2}{2m}G(\mathbf{x},0^-)\Big|_{\mathbf{x}=0}\end{aligned} \quad \text{(6.72)}$$

[2] According to an aprocryphal story, the relativistic counterpart of this notion, that positrons are electrons travelling backwards in time, was invented by Richard Feynman while a graduate student of John Wheeler at Princeton. Wheeler was strict, allowing his graduate students precisely half an hour of discussion a week, employing a chess clock as a timer at the meeting. Wheeler treated Feynman no differently and when the alloted time was up, he stopped the clock and announced that the session was over. At their second meeting, Feynman apparently arrived with his own clock, and at the end of the half hour, Feynman stopped his own clock to announce that his advisor, Wheeler's time was up. During this meeting they discussed the physics of positrons and Feynman came up with the idea that that a positron was an electron travelling backwards in time and that there might only be one electron in the whole universe, threading backwards and forwards in time. To mark the discovery, at the third meeting Dick Feynman arrived with a modified clock which he had fixed to start at 30 minutes and run backwards to zero!

Example 6.2: By relating the particle density and kinetic energy density to one-particle Green's function to the particle density, calculate the particle and kinetic energy density of particles in a degenerate Fermi liquid.

Solution: We begin by writing $\langle \hat{\rho}(x)\rangle = -i(2S+1)G(\vec{0},0^-)$. Writing this out explicitly we obtain

$$\langle \rho(x)\rangle = (2S+1)\int \frac{d^3k}{(2\pi)^3}\left[\int \frac{d\omega}{2\pi i}e^{i\omega\delta}\frac{1}{\omega-\epsilon_{\mathbf{k}}+i\delta_{\mathbf{k}}}\right] \tag{6.73}$$

where the convergence factor appears because we are evaluating the Green's function at a small negative time $-\delta$. We have explicitly separated out the frequency and momentum integrals. The poles of the propagator are at $\omega = \epsilon_{\mathbf{k}} - i\delta$ if $k > k_F$, but at $\omega = \epsilon_{\mathbf{k}} + i\delta$ if $k < k_F$, as illustrated in Fig. 6.4. The convergence factor means that we can calculate the complex integral using Cauchy's theorem by completing the contour in the upper half complex plane, where the integrand dies away exponentially. The pole in the integral will only pick up those poles associated with states below the Fermi energy, so that

$$\int \frac{d\omega}{2\pi i}e^{i\omega\delta}\frac{1}{\omega-\epsilon_{\mathbf{k}}+i\delta_{\mathbf{k}}} = \theta_{k_F-|\mathbf{k}|} \tag{6.74}$$

and hence

$$\rho = (2S+1)\int_{k<k_F}\frac{d^3k}{(2\pi)^3} = (2S+1)\frac{V_F}{(2\pi)^3} \tag{6.75}$$

In a similar way, the kinetic energy density is written

$$\begin{aligned}\langle T(x)\rangle &= (2S+1)\int \frac{d^3k}{(2\pi)^3}\frac{\hbar^2k^2}{2m}\left[\int \frac{d\omega}{2\pi i}e^{i\omega\delta}\frac{1}{\omega-\epsilon_{\mathbf{k}}+i\delta_{\mathbf{k}}}\right]\\ &= (2S+1)\int_{k<k_F}\frac{d^3k}{(2\pi)^3}\frac{\hbar^2k^2}{2m} = \frac{3}{5}\epsilon_F\rho\end{aligned} \tag{6.76}$$

6.2.2 Green's function for free Bosons

As a second example, let us examine the Green's function of a gas of non-interacting bosons, described by

$$H = \sum_{\mathbf{q}}\omega_{\mathbf{q}}[b^\dagger_{\mathbf{q}}b_{\mathbf{q}} + \frac{1}{2}] \tag{6.77}$$

where physical field operator is related to a sum of creation and annihilation operators:

$$\begin{aligned}\phi(x) &= \int_q \phi_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{x}}\\ \phi_{\mathbf{q}} &= \sqrt{\frac{\hbar}{2m\omega_{\mathbf{q}}}}[b_{\mathbf{q}} + b^\dagger_{-\mathbf{q}}]\end{aligned} \tag{6.78}$$

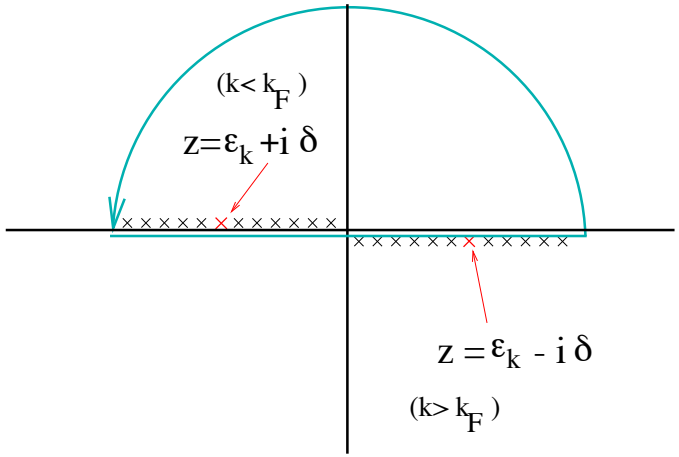


Figure 6.4: Showing how the path of integration in (6.74) picks up the pole contributions from the occupied states beneath the Fermi surface.

Since there are no bosons present in the ground-state, boson destruction operators annihilate the ground-state $|\phi\rangle$. The only terms contributing to the Green function are then

$$\begin{aligned}-i\langle\phi|Tb_{\mathbf{q}}(t)b^\dagger_{\mathbf{q}}(0)|\phi\rangle &= -i\theta(t)e^{-i\omega_{\mathbf{q}}t},\\ -i\langle\phi|Tb^\dagger_{-\mathbf{q}}(t)b_{-\mathbf{q}}(0)|\phi\rangle &= -i\theta(-t)e^{i\omega_{\mathbf{q}}t},\end{aligned} \tag{6.79}$$

so that

$$D(\mathbf{q},t) = -i\langle\phi|\phi(\mathbf{q},t)\phi(-\mathbf{q},t)|\phi\rangle = -i\frac{\hbar}{2m\omega_{\mathbf{q}}}[\theta(t)e^{-i\omega_{\mathbf{q}}t} + \theta(-t)e^{i\omega_{\mathbf{q}}t}] \tag{6.80}$$

If we Fourier transform this quantity, we obtain the boson propgator,

$$\begin{aligned}D(\mathbf{q},\nu) &= \int_{-\infty}^{\infty}dte^{-\delta|t|+i\nu t}D(\mathbf{q},t)\\ &= -i\frac{\hbar}{2m\omega_{\mathbf{q}}}\left[\frac{1}{\delta-i(\nu-\omega_{\mathbf{q}})} + \frac{1}{\delta+i(\nu-\omega_{\mathbf{q}})}\right]\end{aligned} \tag{6.81}$$

or

$$D(\mathbf{q},\nu) = \frac{\hbar}{2m\omega_{\mathbf{q}}}\left[\frac{2\omega_{\mathbf{q}}}{\nu^2-(\omega_{\mathbf{q}}-i\delta)^2}\right], \qquad \text{Bose propagator} \tag{6.82}$$

Remarks:

- Note that the bose propagator has two poles at $\nu = \pm(\omega - i\delta)$. You can think of the bose propagator as a sum of two terms, one involving a boson emission, that propagates forwards in time from the emitter, a second involving boson absorption that propagates backwards in time from the absorber,

$$D(\mathbf{q},\nu) = \frac{\hbar}{2m\omega_{\mathbf{q}}}\left[\overbrace{\frac{1}{\nu-(\omega_{\mathbf{q}}-i\delta)}}^{\text{emission}} + \overbrace{\frac{1}{-\nu-(\omega_{\mathbf{q}}-i\delta)}}^{\text{absorption}}\right] \tag{6.83}$$

- We shall shortly see that amplitude to absorb and emit bosons by propagating fermions is directly related to the Boson propagator. For example, when there is an interaction of the form

$$H_{int} = g\int d^3x\phi(\mathbf{x})\rho(\mathbf{x}) \tag{6.84}$$

The exchange of virtual bosons between particles gives rise to *retarded* interactions,

$$V(\mathbf{q},t-t') = \frac{g^2}{\hbar}D(\mathbf{q},t-t'), \tag{6.85}$$

whereby a passing fermion produces a the potential change in the environment which lasts a characteristic time $\Delta\tau \sim 1/\omega_o$ where ω_o is the characteristic value of $\omega_{\mathbf{q}}$. From the Fourier transform of this expression, you can see that the time average of this interaction, proportional to $D(\mathbf{q},\nu=0) = -\frac{\hbar}{m\omega_q^2}$ is negative: i.e. the virtual exchange of a spinless boson mediates an attractive interaction.

6.3 Adiabatic concept

The adiabatic concept is one of the most valuable concepts in many body theory. What does it mean to understand a many body problem when we can never, except in the most special cases, expect to solve the problem exactly? The adiabatic concept provides an answer to this question.

Suppose we are interested in a many body problem with Hamiltonian H, with ground-state $|\Psi_g\rangle$ which we can not solve exactly. Instead we can often solve a simplified version of the many body Hamiltonian H_o where the ground-state $|\tilde{\Psi}_g\rangle$ has the same *symmetry* as $|\Psi_g\rangle$. Suppose we start in

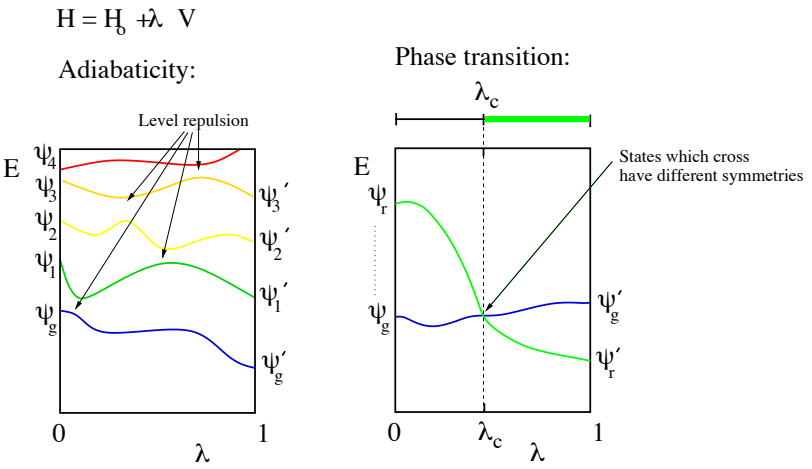


Figure 6.5: Illustrating the evolution of the Hilbert space as the Hamiltonian is adiabatically evolved. In the first case, the ground-state can be adiabatically evolved all the way to $\lambda = 1$. In the second case, a phase transition occurs at $\lambda = \lambda_c$, where a previously excited state, with a different symmetry to the ground-state crosses below the ground-state.

the ground-state $|\tilde{\Psi}_g\rangle$, and now slowly evolve the Hamiltonian from H_o to H, i.e, if $\hat{V} = H - H_o$, we imagine that the state time-evolves according to the Hamiltonian

$$\begin{aligned} H(t) &= H_o + \lambda(t)V \\ \lambda(t) &= e^{-|t|\delta} \end{aligned} \tag{6.86}$$

where δ is arbitrarily small.

As we adiabatically evolve the system, the ground-state, and excited states will evolve, as shown in Fig. 6.5. In such an evolution process, the energy levels will typically show "energy level repulsion". If any two levels get too close together, matrix elements between the two states will cause them to repel one-another. However, it is possible for states of different symmetry to cross, because selection rules prevent them from mixing. Sometimes, such an adiabatic evolution will lead to "level crossing", whereby at $\lambda = \lambda_c$ when some excited state ψ_r with different symmetry to the ground-state, crosses to a lower energy than the ground-state. Such a situation leads to "spontaneous symmetry breaking". A simple example is when a Ferromagnetic ground-state becomes stabilized by interactions.

In general however, if there is no symmetry changing phase transition as the interaction V is turned on, the procedure of adiabatic evolution, can be used to turn on "interactions", and to evolve

the ground-state from $\tilde{\Psi}_g$ to Ψ_g.

These ideas play a central role in the development of perturbation theory and Feynman diagrams. They are however also of immense qualitative importance, for the physics of adiabatically related ground-states is equivalent. Adiabatic evolution defines an equivalence class of ground-states with the same qualitative physics. The adiabatic principle was first employed with great success in the fifties. Gell Mann and Low used it to prove their famous relation linking non-interacting, and interacting Green's functions[1]. Later in the fifties, Landau[2, 3, 4] used the adiabatic idea in a brilliantly qualitative fashion, to formulate his theory of interacting Fermi liquids, which we examine in detail in the next chapter.

6.3.1 Gell-Man Low Theorem

Suppose we gradually turn on, and later, gradually turn- off an interaction V so that

$$V(t) = e^{-\epsilon|t|}V(0) \tag{6.87}$$

acquires its full magnetitude at t=0 and vanishes in the distant past and in the far-future. The quantity $\tau_A = \epsilon^{-1}$ sets the characteristic "switch-on time" for the process. Adiabaticity requires that we ultimately let $\epsilon \to 0$, sending the switch-on time to infinity $\tau_A \to \infty$. When we start out at $t = -\infty$, the ground-state is $|-\infty\rangle$, and the interaction and Heisenberg representations coincide. If we now evolve to the present in the Heisenberg representation, the states do not evolve, so the ground-state is unchanged

$$|\phi\rangle_H \equiv |-\infty\rangle, \tag{6.88}$$

and all the interesting physics of the interaction V is encoded in the the operators. We would like to calculate the correlation or Green's functions of a set of observables in the fully interacting system. The Gell-Mann Low theorem enables us to relate the Green's function of the interacting system to the Green's functions of the non-interacting system at $t = -\infty$. The key result is

$$\begin{aligned} \langle\phi|TA(t_1)B(t_2)\dots R(t_r)|\phi\rangle_H &= \langle+\infty|TS[\infty,-\infty]A(t_1)B(t_2)\dots R(t_r)|-\infty\rangle_I \\ S[\infty,-\infty] &= T\exp\Big[-i\int_{-\infty}^{\infty}V(t')dt'\Big] \end{aligned} \tag{6.89}$$

where the subscript H and I indicate that the operators, and states are to be evaluated in the Heisenberg and interaction representations, respectively. The state $|+\infty\rangle = S(\infty,-\infty)|-\infty\rangle$ corresponds to the ground-state, in the interaction representation in the distant future. If adiabaticity holds, then the process of slowly turning on, and then turning off the interaction, will return the system to its original state, up to a phase, so that $|+\infty\rangle = e^{2i\delta}|-\infty\rangle$. We can then write $e^{2i\delta} = \langle-\infty|\infty\rangle$, so that so that

$$\langle+\infty| = e^{-2i\delta}\langle-\infty| = \frac{\langle-\infty|}{\langle-\infty|+\infty\rangle} \tag{6.90}$$

and the Gell-Mann Low formula becomes

$$\langle\phi|TA(t_1)B(t_2)\dots R(t_r)|\phi\rangle_H = \frac{\langle-\infty|TS[\infty,-\infty]A(t_1)B(t_2)\dots R(t_r)|-\infty\rangle_I}{\langle-\infty|S[\infty,-\infty]|-\infty\rangle} \tag{6.91}$$

Remarks:

- With the Gell-Mann Low relation, we relate the Green's function of a set of complex operators in an interacting system, to a Green's function of a set of simple operators multiplied by the S-matrix.
- The Gell-Mann Low relation is the starting point for the Feynman diagram expansion of Green's functions. When we expand the S-matrix as a power-series in V, each term in the expansion can be written as an integral over Green's functions of the non-interacting problem. Each of these terms corresponds to a particular Feynman diagram.
- When we expand the vacuum expectation value of the S-matrix, we will see that this leads to "Linked Cluster" diagrams.

Proof: To prove this result, let $U(t) = S(t,-\infty)$ be the time-evolution operator for the interaction representation. Since the interaction, and Heisenberg states coincide at $t = -\infty$, and $|\psi_H\rangle$ does not evolve with time,

$$|\psi_I(t)\rangle = U(t)|\psi_H\rangle \tag{6.92}$$

Since $U(t)A_H(t)|\psi_H\rangle = A_I(t)|\psi_I(t)\rangle = A_I(t)U(t)|\psi_H\rangle$, the relation between operators in the two representations must be

$$A_H(t) = U^\dagger(t)A_I(t)U(t) \tag{6.93}$$

Suppose $t_1 > t_2 > t_3 \dots t_r$, then using this relation we may write

$$\langle\phi|A(t_1)\dots R(t_r)|\phi\rangle_H = \langle-\infty|U^\dagger(t_1)A_I(t_1)\overbrace{U(t_1)U^\dagger(t_2)}^{S(t_1,t_2)}\dots\overbrace{U(t_{r-1})U^\dagger(t_r)}^{S(t_{r-1},t_r)}R_I(t_r)U(t_r)|-\infty\rangle$$

where we have identified $|\phi\rangle_H \equiv |-\infty\rangle$. Now $S(t_1,t_2) = U(t_1)U^\dagger(t_2)$ is the operator that time evolves the states of the interaction representation, so we may rewrite the above result as

$$\langle 0|A(t_1)\dots R(t_r)|0\rangle_H = \langle-\infty|\overbrace{U^\dagger(t_1)}^{S^\dagger(t_1,-\infty)}A_I(t_1)S(t_1,t_2)\dots S(t_{r-1},t_r)R_I(t_r)\overbrace{U(t_r)}^{S(t_r,-\infty)}|-\infty\rangle$$

where we have replaced $U(t) \to S(t,-\infty)$. Now $S(\infty,t_1)S(t_1,-\infty)|-\infty\rangle = |\infty\rangle$ and since S is a unitary matrix, $S^\dagger(\infty,t_1)S(\infty,t_1) = 1$, so multiplying both sides by $S^\dagger(\infty,t_1)$, $S(t_1,-\infty)|-\infty\rangle = S^\dagger(\infty,t_1)|\infty\rangle$ and by taking its complex conjugate,

$$\langle-\infty|S^\dagger(t_1,-\infty) = \langle\infty|S(\infty,t_1) \tag{6.94}$$

Inserting this into the above expression gives,

$$\langle 0|A(t_1)\ldots R(t_r)|0\rangle_H = \langle +\infty|S(\infty,t_1)A_I(t_1)S(t_1,t_2)\ldots S(t_{r-1},t_r)R_I(t_r)S(t_r,-\infty)|-\infty\rangle$$

Finally, since we assumed $t_1 > t_2 > \ldots t_r$, we can write,

$$\langle\phi|T[A(t_1)\ldots R(t_r)]|\phi\rangle_H = \langle +\infty|T[S(\infty,-\infty)A_I(t_1)B_I(t_2)\ldots R_I(t_r)]|-\infty\rangle \tag{6.95}$$

Although we proved this expression for a particular time-ordering, it is clear that if we permute the operators the time-ordering will always act to time-order both sides, and thus this expression holds for an arbitary time-ordering of operators.

6.3.2 Generating Function for Free fermions

The generating function derived for the harmonic oscillator can be generalized to free fermions by the use of "anticommuting" or Grassman numbers η and η. The simplest model is

$$\left.\begin{array}{rcl} H &=& \epsilon c^\dagger c \\ V(t) &=& \bar\eta(t)c(t) + c^\dagger(t)\eta(t)\end{array}\right\} \tag{6.96}$$

The corresponding Generating functional is given by

$$\begin{array}{rcl} S[\bar\eta,\eta] = \langle\phi|T\exp\left(-i\int dt\left[\bar\eta(t)c(t)+c^\dagger(t)\eta(t)\right]\right)|\phi\rangle &=& \exp\left[-i\int d1d2\bar\eta(1)G(1-2)\eta(2)\right] \\ G(1-2) &=& -i\langle\phi|Tc(1)c^\dagger(2)|\phi\rangle \end{array} \tag{6.97}$$

where $|\phi\rangle$ is the ground-state for the non-interacting Hamiltonian. To prove this result, we use the same method as used for the harmonic oscillator. As before we split up the S matrix into N discrete time-slices, writing

$$S_N = e^{A_N - A^\dagger{}_N}\times\ldots e^{A_r - A^\dagger{}_r}\times\ldots e^{A_1 - A^\dagger{}_1} \tag{6.98}$$

where

$$\begin{array}{rcl} A_r &=& \bar\eta(t_r)(-ice^{-i\epsilon t_r})\Delta t, \\ A^\dagger{}_r &=& \eta(t_r)(ic^\dagger e^{i\epsilon t_r})\Delta t. \end{array} \tag{6.99}$$

The next step requires a little care, for when $\epsilon < 0$, $|\phi\rangle = c^\dagger|0\rangle$ is the vacuum for holes $h = c^\dagger$, rather than particles, so that in this case we need to "anti-normal order" the S matrix. Carrying out the ordering process, we obtain

$$S_N = \left\{\begin{array}{ll} e^{-\sum_r A^\dagger{}_r}e^{\sum_r A_r}\exp\left[-\sum_{r\geq s}[A_r,A^\dagger{}_s](1-\frac{1}{2}\delta_{rs})\right] & (\epsilon>0) \\ e^{\sum_r A_r}e^{-\sum_r A^\dagger{}_r}\exp\left[\sum_{r\leq s}[A_r,A^\dagger{}_s](1-\frac{1}{2}\delta_{rs})\right] & (\epsilon<0)\end{array}\right. \tag{6.100}$$

When we take the expectation value $\langle\phi|S_N|\phi\rangle$, the first term in these expressions gives unity. Calculating the commutators, in the exponent, we obtain

$$\begin{array}{rcl} [A_r, A^\dagger{}_s] &=& \Delta t^2[\bar\eta(t_r)c, c^\dagger\eta(t_s)]e^{-i\epsilon(t_r-t_s)} \\ &=& \Delta t^2\bar\eta(t_r)\{c,c^\dagger\}\eta(t_s)e^{-i\epsilon(t_r-t_s)} \\ &=& \Delta t^2\bar\eta(t_r)\eta(t_s)]e^{-i\epsilon(t_r-t_s)}. \end{array} \tag{6.101}$$

(Notice how the anticommuting property of the Grassman variables $\bar\eta(t_r)\eta(t_s) = -\eta(t_s)\bar\eta(t_r)$ means that we can convert a commutator of $[A_r, A_s]$ into an anticommutator $\{c, c^\dagger\}$.) Next, that taking the limit $N\to\infty$, we obtain

$$S[\bar\eta,\eta] = \left\{\begin{array}{ll} \exp\left[-\int_{-\infty}^{\infty} dtdt'\bar\eta(t)\theta(t-t')\eta(t')e^{-i\epsilon(t-t')}\right] & (\epsilon>0) \\ \exp\left[\int_{-\infty}^{\infty} d\tau d\tau'\bar\eta(\tau)\theta(t'-t)\eta(\tau')e^{-i\epsilon(t-t')}\right] & (\epsilon<0)\end{array}\right. \tag{6.102}$$

By introducing the Green function,

$$G(t) = -i\left[(1-f(\epsilon))\theta(t) - f(\epsilon))\theta(-t)\right]e^{-i\epsilon t}$$

we can compactly combine these two results into the final form

$$S(t_2,t_1) = \exp\Big[-i\int_{-\infty}^{\infty} dtdt'\bar\eta(t)G(t-t')\eta(t')\Big]. \tag{6.103}$$

A more heuristic derivation however, is to recognize that derivatives of the generating functional bring down Fermi operators inside the time-ordered exponential,

$$\begin{array}{rcl} i\frac{\delta}{\delta\eta(t)}\langle\phi|T\hat S\ldots|\phi\rangle &=& \langle\phi|T\hat S\, c^\dagger(t)\ldots|\phi\rangle \\ i\frac{\delta}{\delta\bar\eta(t)}\langle\phi|T\hat S\ldots|\phi\rangle &=& \langle\phi|T\hat S\, c(t)\ldots|\phi\rangle \end{array} \tag{6.104}$$

where $\hat S = T\exp\left[-i\int dt'\left(\bar\eta(t')c(t') + c^\dagger(t')\eta(t')\right)\right]$ so that inside the expectation value,

$$\begin{array}{rcl} i\frac{\delta}{\delta\eta(t)} &\equiv& c^\dagger(t) \\ i\frac{\delta}{\delta\bar\eta(t)} &\equiv& c(t), \end{array} \tag{6.105}$$

and

$$i\frac{\delta\ln S}{\delta\eta(1)} = \frac{\langle\phi|Tc^\dagger(1)\hat S|\phi\rangle}{\langle\phi|\hat S|\phi\rangle} \equiv \langle c^\dagger(1)\rangle, \tag{6.106}$$

where $\hat S = T\exp\left[-i\int V(t')dt'\right]$. Here, we have used the Gell-Mann Low theorem to identify the quotient above as the expectation value for $c^\dagger(1)$ in the presence of the source terms. Differentiating one more time,

$$(i)^2\frac{\delta^2\ln S[\bar\eta,\eta]}{\delta\bar\eta(2)\delta\eta(1)} = \frac{\langle\phi|Tc(2)c^\dagger(1)\hat S|\phi\rangle}{\langle\phi|\hat S|\phi\rangle} - \frac{\langle\phi|Tc(2)\hat S|\phi\rangle}{\langle\phi|\hat S|\phi\rangle}\frac{\langle\phi|Tc^\dagger(1)\hat S|\phi\rangle}{\langle\phi|\hat S|\phi\rangle}$$

$$\begin{aligned} &= \langle Tc(2)c^\dagger(1)\rangle - \langle c(2)\rangle\langle c^\dagger(1)\rangle \\ &= \langle T\delta c(2)\delta c^\dagger(1)\rangle. \end{aligned} \tag{6.107}$$

This quantity describes the variance in the fluctuations $\delta c^{(\dagger)}(2) \equiv c^{(\dagger)}(2) - \langle c^{(\dagger)}(2)\rangle$ of the fermion field about their average value. When the source terms η and $\bar\eta$ are introduced, they induce a finite (Grassman) expectation value of the fields $\langle c(1)\rangle$ and $\langle c^\dagger(1)\rangle$ but the absence of interactions between the modes mean they won't change the amplitude of fluctuations about the mean, so that

$$(i)^2\frac{\delta^2 \ln S[\bar\eta,\eta]}{\delta\bar\eta(2)\delta\eta(1)} = \langle Tc(1)c^\dagger(2)\rangle\big|_{\eta,\,\bar\eta=0} = iG(1-2),$$

and we can then deduce that

$$\ln S[\bar\eta,\eta] = -i\int d1d2\bar\eta(2)G(2-1)\eta(1). \tag{6.108}$$

There is no constant term, because $S = 1$ when the source terms are removed, and we arrive back at (6.97).

The generalization of the generating functional to a gas of Fermions with many one-particle states is just a question of including an appropriate sum over one-particle states, i.e

$$\left.\begin{aligned} H &= \textstyle\sum_\lambda \epsilon_\lambda c^\dagger{}_\lambda c_\lambda \\ V(t) &= \textstyle\sum_\lambda \bar\eta_\lambda(t)c_\lambda(t) + c_\lambda{}^\dagger(t)\eta_\lambda(t) \end{aligned}\right\} \tag{6.109}$$

The corresponding Generating functional is given by

$$\begin{aligned} S[\bar\eta,\eta] &= \langle\phi|T\exp\left[-i\int d1\sum_\lambda \bar\eta_\lambda(1)c_\lambda(1) + c_\lambda{}^\dagger(1)\eta_\lambda(1)\right]|\phi\rangle \\ &= \exp\left[-i\sum_\lambda\int d1d2\bar\eta_\lambda(1)G_\lambda(1-2)\eta_\lambda(2)\right] \\ G_\lambda(1-2) &= -i\langle\phi|Tc_\lambda(1)c^\dagger{}_\lambda(2)|\phi\rangle \end{aligned} \tag{6.110}$$

Example 6.3: Show using the generating function, that in the presence of a source term,

$$\langle c_\lambda(1)\rangle = \int d2G_\lambda(1-2)\eta_\lambda(2). \tag{6.111}$$

Solution: Taking the (functional) derivative of (6.110) with respect to η_λ, from the left-hand side of (6.110), we obtain

$$\frac{\delta S[\bar\eta,\eta]}{\delta\bar\eta_\lambda(1)} = -i\langle\phi|Tc_\lambda(1)\exp\left[-i\int dtV(t)\right]|\phi\rangle \tag{6.112}$$

so that

$$i\frac{\delta\ln S[\bar\eta,\eta]}{\delta\bar\eta_\lambda(1)} = \frac{i}{S[\bar\eta,\eta]}\frac{\delta S[\bar\eta,\eta]}{\delta\bar\eta_\lambda(1)} = \frac{\langle\phi|Tc_\lambda(1)\exp\left[-i\int dtV(t)\right]|\phi\rangle}{\langle\phi|T\exp\left[-i\int dtV(t)\right]|\phi\rangle} = \langle c_\lambda(1)\rangle. \tag{6.113}$$

Now taking the logarithm of the right-hand side of (6.110), we obtain

$$i\ln S[\bar\eta,\eta] = \sum_\lambda\int d1d2\bar\eta_\lambda(1)G_\lambda(1-2)\eta_\lambda(2) \tag{6.114}$$

so that

$$i\frac{\delta\ln S[\bar\eta,\eta]}{\delta\bar\eta_\lambda(\tau)} = \int d2G_\lambda(1-2)\eta_\lambda(2) \tag{6.115}$$

Combining (6.113) with (6.115) we obtain the final result

$$\langle c_\lambda(1)\rangle = \int d2G_\lambda(1-2)\eta_\lambda(2) \tag{6.116}$$

6.3.3 The Spectral Representation

In the non-interacting Fermi liquid, we saw that the propagator contained a single pole, at $\omega = \epsilon_{\mathbf{k}}$. What happens to the propagator when we turn on the interactions? Remarkably it retains its same general analytic structure, excepting that now, the single pole divides into a plethora of poles, each one corresponding to an excitation energy for adding, or removing a particle from the ground-state. The general result, is that

$$G(\mathbf{k},\omega) = \sum_\lambda \frac{|M_\lambda(\mathbf{k})|^2}{\omega - \epsilon_\lambda + i\delta_\lambda} \tag{6.117}$$

where $\delta_\lambda = \delta\text{sign}(\epsilon_\lambda)$ and the total pole strength

$$\sum_\lambda |M_\lambda(\mathbf{k})|^2 = 1 \tag{6.118}$$

is unchanged. Notice how the positive energy poles of the Green function are below the real axis at $\epsilon_\lambda - i\delta$, while the negative energy poles are below the real axis, preserving the pole structure of the non-interacting Green's function.

If the ground-state is an N particle state, then the state $|\lambda\rangle$ is either an $N+1$, or $N-1$ particle state. The poles of the Green function are given by related to the excitation energies $E_\lambda - E_g > 0$ according to

$$\epsilon_\lambda = \begin{cases} E_\lambda - E_g > 0 & (|\lambda\rangle \in |N+1\rangle) \\ -1\times(E_\lambda - E_g) < 0 & (|\lambda\rangle \in |N-1\rangle) \end{cases}, \tag{6.119}$$

and the corresponding matrix elements are

$$M_\lambda(\mathbf{k}) = \begin{cases} \langle\lambda|c^\dagger_{\mathbf{k}\sigma}|\phi\rangle, & (|\lambda\rangle \in |N+1\rangle), \\ \\ \langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle, & (|\lambda\rangle \in |N-1\rangle). \end{cases} \tag{6.120}$$

Notice that the excitation energies $E_\lambda - E_g > 0$ are always positive, so $\epsilon_\lambda > 0$ measures the energy to add and electron, while $\epsilon_\lambda < 0$ measures $-1\times$ the energy to create a hole state.

In practice, the poles in the interacting Green function blur into a continuum of excitation energies, with an infinitesimal separation. To deal with this situation, we define a quantity known as the spectral function, given by the imaginary part of the Green's function,

$$A(\mathbf{k},\omega) = \frac{1}{\pi}\mathrm{Im}G(\mathbf{k},\omega - i\delta), \qquad \textbf{Spectral Function} \tag{6.121}$$

By shifting the frequency ω by a small imaginary part which is taken to zero at the end of the calculation, overriding the δ_λ in (6.117), all the poles of $G(\mathbf{k},\omega - i\delta)$ are moved above the real axis. Using Cauchy's principle part equation, $1/(x - i\delta) = P(1/x) + i\pi\delta(x)$, where P denotes the principal part, we can use the spectral representation (6.117) to write

$$\begin{aligned} A(\mathbf{k},\omega) &= \sum_\lambda |M_\lambda(\mathbf{k})|^2\delta(\omega - \epsilon_\lambda) \\ &= \sum_\lambda \Big[|\langle\lambda|c^\dagger_{\mathbf{k}\sigma}|\phi\rangle|^2\theta(\omega) + \langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2\theta(-\omega)\Big]\delta(|\omega| - (E_\lambda - E_g)) \end{aligned} \tag{6.122}$$

where now, the normalization of the pole-strengths means that

$$\int_{-\infty}^{\infty} A(\mathbf{k},\omega)d\omega = \sum_\lambda |M_\lambda(\mathbf{k})|^2 = 1 \tag{6.123}$$

Since the excitation energies are positive, $E_\lambda - E_g > 0$ from (6.119) it follows that ϵ_λ is positive for electron states and negative for hole states, so

$$A(\mathbf{k},\omega) = \theta(\omega)\rho_e(\mathbf{k},\omega) + \theta(-\omega)\rho_h(\mathbf{k},-\omega) \tag{6.124}$$

where

$$\rho_e(\omega) = \sum_\lambda |\langle\lambda|c^\dagger_{\mathbf{k}\sigma}|\phi\rangle|^2\delta(\omega - (E_\lambda - E_g)) \qquad (\omega > 0) \tag{6.125}$$

and

$$\rho_h(\omega) = \sum_\lambda |\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2\delta(\omega - (E_g - E_\lambda)) \qquad (\omega > 0) \tag{6.126}$$

are the spectral functions for adding or holes of energy ω to the system respectively. To a good approximation, in high energy spectroscopy, $\rho_{e,h}(\mathbf{k},\omega)$ is directly proportional to the cross-section for adding, or removing an electron of energy $|\omega|$ to the material. Photoemission and inverse photoemission experiments can, in this way, be used to directly measure the spectral function of electronic systems.

To derive this spectral decomposition, we suppose that we know the complete Hilbert space of energy eigenstates $\{|\lambda\rangle\}$. By injecting the completeness relation $\sum|\lambda\rangle\langle\lambda| = 1$ between the creation and annihilation operators in the Green's function, we can expand it as follows

$$\begin{aligned} G(\mathbf{k},t) &= -i\Big[\langle\phi|c_{\mathbf{k}\sigma}(t)c^\dagger_{\mathbf{k}\sigma}(0)|\phi\rangle\theta(t) - \langle\phi|c^\dagger_{\mathbf{k}\sigma}(0)c_{\mathbf{k}\sigma}(t)|\phi\rangle\theta(-t)\Big] \\ &= -i\sum_\lambda\Big[\langle\phi|c_{\mathbf{k}\sigma}(t)\overbrace{|\lambda\rangle\langle\lambda|}^{=1}c^\dagger_{\mathbf{k}\sigma}(0)|\phi\rangle\theta(t) - \langle\phi|c^\dagger_{\mathbf{k}\sigma}(0)\overbrace{|\lambda\rangle\langle\lambda|}^{=1}c_{\mathbf{k}\sigma}(t)|\phi\rangle\theta(-t)\Big] \end{aligned}$$

By using energy eigenstates, we are able to write

$$\begin{aligned} \langle\phi|c_{\mathbf{k}\sigma}(t)|\lambda\rangle &= \langle\phi|e^{iHt}c_{\mathbf{k}\sigma}e^{-iHt}|\lambda\rangle = \langle\phi|c_{\mathbf{k}\sigma}|\lambda\rangle e^{i(E_g - E_\lambda)t} \\ \langle\lambda|c_{\mathbf{k}\sigma}(t)|\phi\rangle &= \langle\lambda|e^{iHt}c_{\mathbf{k}\sigma}e^{-iHt}|\phi\rangle = \langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle e^{i(E_\lambda - E_g)t} \end{aligned} \tag{6.127}$$

Notice that the first term involves adding a particle of momentum $\mathbf{k}$, spin σ, so that the state $|\lambda\rangle = |N+1;\mathbf{k}\sigma\rangle$ is an energy eigenstate with $N+1$ particles, momentum $\mathbf{k}$ and spin σ. Similarly, in the second matrix element, a particle of momentum $\mathbf{k}$, spin σ has been *subtracted*, so that $|\lambda\rangle = |N-1;-\mathbf{k}\ -\sigma\rangle$. We can thus write the Green's function in the form:

$$G(\mathbf{k},t) = -i\sum_\lambda\Big[|\langle\lambda|c^\dagger_{\mathbf{k}\sigma}|\phi\rangle|^2e^{-i(E_\lambda - E_g)t}\theta(t) - |\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2e^{-i(E_g - E_\lambda)t}\theta(-t)\Big],$$

where we have simplified the expression by writing $\langle\phi|c_{\mathbf{k}\sigma}|\lambda\rangle = \langle\lambda|c^\dagger_{\mathbf{k}\sigma}|\phi\rangle^*$ and $\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle = \langle\phi|c^\dagger_{\mathbf{k}\sigma}|\lambda\rangle^*$. This has precisely the same structure as a non-interacting Green's function, except that $\epsilon_{\mathbf{k}} \to E_\lambda - E_g$ in the first term, and $\epsilon_{\mathbf{k}} \to E_g - E_\lambda$ in the second term. We can use this observation to carry out the Fourier transform, whereapon

$$G(\mathbf{k},\omega) = \sum_\lambda\left[\frac{|\langle\lambda|c^\dagger_{\mathbf{k}\sigma}|\phi\rangle|^2}{\omega - (E_\lambda - E_g) + i\delta} + \frac{|\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2}{\omega - (E_g - E_\lambda) - i\delta}\right]$$

which is the formal expansion of (6.117).

To show that the total pole-strength is unchanged by interactions, we expand the sum over pole strengths, and then use completeness again, as follows

$$\begin{aligned} \sum_\lambda |M_\lambda(\mathbf{k})|^2 &= \sum_\lambda |\langle\lambda|c^\dagger_{\mathbf{k}\sigma}|\phi\rangle|^2 + |\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2 \\ &= \sum_\lambda \langle\phi|c_{\mathbf{k}\sigma}\overbrace{|\lambda\rangle\langle\lambda|}^{=1}c^\dagger_{\mathbf{k}\sigma}|\phi\rangle + \langle\phi|c^\dagger_{\mathbf{k}\sigma}\overbrace{|\lambda\rangle\langle\lambda|}^{=1}c_{\mathbf{k}\sigma}|\phi\rangle \\ &= \langle\phi|\overbrace{\{c_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}\sigma}\}}^{=1}|\phi\rangle = 1 \end{aligned} \tag{6.128}$$

Example 6.4: Using the spectral decomposition, show that the momentum distribution function in the ground-state of a translationally invariant system of fermions is given the integral over the "filled" states

$$\sum_\sigma \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle = (2S+1)\int_{-\infty}^0 d\omega A(\mathbf{k},\omega)$$

Solution: Let us first write the occupancy in terms of the one-particle Green's function evaluated at time $t = 0^-$

$$\langle n_{\mathbf{k}\sigma}\rangle = \langle\phi|n_{\mathbf{k}\sigma}|\phi\rangle = -i\times -i\langle\phi|Tc_{\mathbf{k}\sigma}(0^-)c^\dagger{}_{\mathbf{k}\sigma}(0)|\phi\rangle = -iG(\mathbf{k},0^-),$$

Now using the spectral representation, (6.128),

$$\langle n_{\mathbf{k}\sigma}\rangle = -iG(\mathbf{k},0^-) = \sum_\lambda |\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2 = \sum_\lambda |M_\lambda(\mathbf{k})|^2\theta(-\epsilon_\lambda)$$

since $|M_\lambda(\mathbf{k})|^2 = |\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2$ for $\epsilon_\lambda < 0$. This is just the sum over the negative energy part of the spectral function. Now since $A(\mathbf{k},\omega) = \sum_\lambda |M_\lambda(\mathbf{k})|^2\delta(\omega-\epsilon_\lambda)$, it follows that at absolute zero,

$$\int_{-\infty}^0 d\omega(\mathbf{k},\omega) = \sum_\lambda |M_\lambda(\mathbf{k})|^2 \overbrace{\int_{-\infty}^0 d\omega\delta(\omega-\epsilon_\lambda)}^{\theta(-\epsilon_\lambda)} = \sum_\lambda |M_\lambda(\mathbf{k})|^2\theta(-\epsilon_\lambda).$$

so that

$$\sum_\sigma \langle n_{\mathbf{k}\sigma}\rangle = (2S+1)\int_{-\infty}^0 \frac{d\omega}{\pi}A(\mathbf{k},\omega).$$

Example 6.5: Show that the zero temperature Green's function can be written in terms of the Spectral function as follows:

$$G(\mathbf{k},\omega) = \int d\epsilon \frac{1}{\omega-\epsilon(1-i\delta)}A(\mathbf{k},\epsilon).$$

Solution: Introduce the relationship $1 = \int d\epsilon\delta(\epsilon-(E_\lambda-E_g))$ and $1 = \int d\epsilon\delta(\epsilon+(E_\lambda-E_g))$ into (6.128) to obtain

$$\begin{aligned} G(\mathbf{k},\omega) &= \int d\epsilon \frac{1}{\omega-\epsilon+i\delta}\sum_\lambda |\langle\lambda|c^\dagger_{\mathbf{k}\sigma}|\phi\rangle|^2\delta(\epsilon-(E_\lambda-E_g)) \\ &+ \int d\epsilon \frac{1}{\omega-\epsilon-i\delta}\sum_\lambda |\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2\delta(\epsilon+(E_\lambda-E_g)). \end{aligned} \quad (6.129)$$

Now in the first term, $\epsilon > 0$, while in the second term, $\epsilon < 0$nn, enabling us to rewrite this expression as

$$G(\mathbf{k},\omega) = \int d\epsilon \frac{1}{\omega-\epsilon(1-i\delta)} \overbrace{\sum_\lambda \left[|\langle\lambda|c^\dagger_{\mathbf{k}\sigma}|\phi\rangle|^2\theta(\epsilon)+|\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2\theta(-\epsilon)\right]\delta(|\epsilon|-(E_\lambda-E_g))}^{A(\mathbf{k},\epsilon)}.$$

giving the quoted result.

6.4 Many particle Green's functions

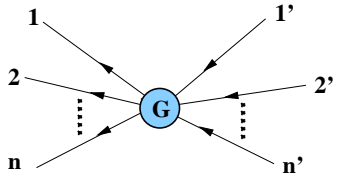
The n-particle Green's function determines the amplitude for n-particles to go from one starting configuration to another:

$$\overbrace{\{1',2'\ldots n'\}}^{\text{initial particle positions}} \xrightarrow{G} \overbrace{\{1,2\ldots n\}}^{\text{final particle positions}} \quad (6.130)$$

where $1' \equiv (\mathbf{x}',t')$, *etc.* and $1 \equiv (\mathbf{x},t)$, *etc.*. The n-particle Green's function is defined as

$$G(1,2,\ldots n;1',2',\ldots n') = (-i)^n\langle\phi|T\psi(1)\psi(2)\ldots\psi(n)\psi^\dagger(n')\ldots\psi^\dagger(1')|\phi\rangle$$

and represented diagramatically as

$G(1,2,\ldots n;1',2',\ldots n') =$ 

(6.131)

In systems without interactions, the n-body Green's function can always be decomposed in terms of the one-body Green's function, a result known as "Wick's theorem". This is because particles propagate without scattering off one-another. Suppose a particle which ends up at $\mathbf{r}$ comes from location P'_r, where P_r is the r-th element of a permutation P of $(1,2,\ldots n)$. The amplitude for this process is

$$G(\mathbf{r}-P'_{\mathbf{r}}) \quad (6.132)$$

and the overall amplitude for all n-particles to go from locations P'_r to positions r is then

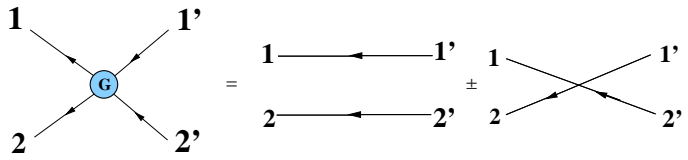
$$\zeta^p G(1-P'_1)G(2-P'_2)\ldots G(n-P'_n) \quad (6.133)$$

where $\zeta = \pm$ for bosons (+) and fermions (-) and p is the number of pairwise permutations required to make the permutation P. This prefactor arises because for fermions, every time we exchange two of them, we pick up a minus sign in the amplitude. Wick's theorem states the physically reasonable result that the n-body Green's function of a non-interacting system is given by the sum of all such amplitudes:

$$G(\mathbf{1},\mathbf{2},\ldots\mathbf{n};\mathbf{1'},\mathbf{2'},\ldots\mathbf{n'}) = \sum \zeta^P \prod_{r=1,n} G(\mathbf{r}-P'_r) \quad (6.134)$$

For example, the two-body Green's function is given by

$$G(\mathbf{1},\mathbf{2}1',\mathbf{2}') = G(\mathbf{1},\mathbf{1}')G(\mathbf{2},\mathbf{2}') \pm G(\mathbf{1},\mathbf{2}')G(\mathbf{2},\mathbf{1}')$$



The process of identifying pairs of initial, and final states in the n-particle Green's function is often referred to as a "contraction". When we contraction two field operators inside a Green's function, we associate an amplitude with the contraction as follows

$$\langle 0|T[\ldots\psi(\mathbf{1})\ldots\psi^\dagger(\mathbf{2})\ldots]|0\rangle \longrightarrow \langle 0|T[\psi(\mathbf{1})\psi^\dagger(\mathbf{2})]|0\rangle = iG(\mathbf{1}-\mathbf{2})$$

$$\langle 0|T[\ldots\psi^\dagger(\mathbf{2})\ldots\psi(\mathbf{1})\ldots]|0\rangle \longrightarrow \langle 0|T[\psi^\dagger(\mathbf{2})\psi(\mathbf{1})]|0\rangle = \pm iG(\mathbf{1}-\mathbf{2})$$

Each product of Green's functions in the Wick-expansion of the propagator is a particular "contraction" of the n-body Green's function, thus

$$\begin{aligned}&(-i)^n\langle 0|T[\psi(\mathbf{1})\psi(\mathbf{2})\ldots\psi(\mathbf{n})\ldots\psi^\dagger(\mathbf{P}'_\mathbf{2})\ldots\psi^\dagger(\mathbf{P}'_\mathbf{1})\ldots\psi^\dagger(\mathbf{P}'_\mathbf{n})]|0\rangle\\ = \;&\zeta^P G(\mathbf{1}-P'_1)G(\mathbf{2}-P'_2)\ldots G(\mathbf{n}-P'_n)\end{aligned} \tag{6.135}$$

where now P is just the number of times the contraction lines cross-one another. Wick's theorem then states that the n-body Green's function is given by the sum over all possible contractions

$$(-i)^n\langle\phi| \;\; T \;\; \psi(1)\psi(2)\ldots\psi^\dagger(n')|\phi\rangle = \sum_{\text{All contractions}} (-i)^n\langle 0|T[\psi(\mathbf{1})\psi(\mathbf{2})\ldots\psi(\mathbf{n})\ldots\psi^\dagger(\mathbf{P}'_\mathbf{2})\ldots\psi^\dagger(\mathbf{P}'_\mathbf{1})\ldots\psi^\dagger(\mathbf{P}'_\mathbf{n})]|0\rangle$$

Example 6.6: Show how the expansion of the generating functional in the absence of interactions can be used to derive Wick's theorem.

6.5 Exercises

1. A particle with $S = 1/2$ is placed in a large magnetic field $\vec{B} = (B_1\cos(\omega t), B_1\sin(\omega t), B_o)$, where $B_o >> B_1$.

   (a) Treating the oscillating part of the Hamiltonian as the interaction, write down the Schrödinger equation in the interaction representation.

   (b) Find $U(t) = \mathrm{T}\exp\left[-iH_{int}(t')dt'\right]$ by whatever method proves most convenient.

   (c) If the particle starts out at time $t = 0$ in the state $S_z = -\frac{1}{2}$, what is the probability it is in this state at time t ?

2. (Optional derivation of bosonic generating functional.) Consider the forced Harmonic oscillator

$$H(t) = \omega b^\dagger b + \bar{z}(t)b + b^\dagger z(t) \tag{6.136}$$

where $z(t)$ and $\bar{z}(t)$ are arbitrary, independent functions of time. Consider the S-matrix

$$S[z,\bar{z}] = \langle 0|\mathrm{T}\hat{S}(\infty,-\infty)|0\rangle = \langle 0|\mathrm{T}\exp\left(-i\int_{-\infty}^{\infty}dt[\bar{z}(t)b(t) + \bar{b}(t)^\dagger z(t)]\right)|0\rangle, \tag{6.137}$$

where $\hat{b}(t)$ denotes $\hat{b}$ in the interaction representation. Consider changing the function $\bar{z}(t)$ by an infinitesimal amount

$$\bar{z}(t) \to \bar{z}(t) + \Delta\bar{z}(t_o)\delta(t-t_o), \tag{6.138}$$

The quantity

$$\lim_{\Delta\bar{z}(t_o)\to 0}\frac{\Delta S[z,\bar{z}]}{\Delta\bar{z}(t_o)} = \frac{\delta S[z,\bar{z}]}{\delta\bar{z}(t_o)}$$

is called the "functional derivative" of S with respect to $\bar{z}$. Using the Gell-Man Lowe formula $\langle\psi(t)|b|\psi(t)\rangle = \frac{\langle 0|T\hat{S}(\infty,-\infty)b(t)|0\rangle}{\langle 0|T\hat{S}(\infty,-\infty)|0\rangle}$ prove the following identity

$$i\delta\ln S[z,\bar{z}]/\delta\bar{z}(t) \equiv \bar{b}(t) = \langle\hat{b}(t)\rangle = \langle\psi(t)|\hat{b}|\psi(t)\rangle. \tag{6.139}$$

(ii) Use the equation of motion to show that

$$\frac{\partial}{\partial t}\bar{b}(t) = i\langle[H(t),\hat{b}(t)]\rangle = -i[\epsilon\bar{b}(t) + z(t)].$$

(iii) Solve the above differential equation to show that

$$\bar{b}(t) = \int_{-\infty}^{\infty}G(t-t')z(t') \tag{6.140}$$

where $G(t-t') = -i\langle 0|T[b(t)b^\dagger(t')]|0\rangle$ is the free Green's function for the harmonic oscillator.

(iv) Use (iii) and (i) together to obtain the fundamental result

$$S[z,\bar{z}] = \exp\left[-i\int_{-\infty}^{\infty} dtdt'\bar{z}(t)G(t-t')z(t')\right] \tag{6.141}$$

3. (Harder problem for extra credit).

Consider a harmonic oscillator with charge e, so that an applied field changes the Hamiltonian $H \to H_o - eE(t)\hat{x}$, where x is the displacement and $E(t)$ the field. Let the system initially be in its ground-state, and suppose a constant electric field E is applied for a time T.

(i) Rewrite the Hamiltonian in the form of a forced Harmonic oscillator

$$H(t) = \omega b^\dagger b + \bar{z}(t)b + b^\dagger z(t) \tag{6.142}$$

and show that

$$z(t) = \bar{z}(t) = \begin{cases} \omega\alpha & (T > t > 0) \\ 0 & (\text{otherwise}) \end{cases}, \tag{6.143}$$

deriving an explicit expression for α in terms of the field E, mass m, and frequency ω of the oscillator.

(ii) Use the explicit form of $S(\bar{z},z)$

$$S[z,\bar{z}] = \exp\left[-i\int_{-\infty}^{\infty} dtdt'\bar{z}(t)G(t-t')z(t')\right] \tag{6.144}$$

where $G(t-t') = -i\langle 0|T[b(t)b^\dagger(t')]|0\rangle$ is the free bosonic Green-function, to calculate the probability $p(T)$ that the system is still in the ground-state after time T. Please express your result in terms of α, ω and T. Sketch the form of $p(T)$ and comment on your result.

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Chapter 7

Landau Fermi Liquid Theory

7.1 Introduction

One of the remarkable features of a Fermi fluid, is its robustness against perturbation. In a typical electron fluid inside metals, the Coulomb energy is comparable with the electron kinetic energy, constituting a major perturbation to the electron motions. Yet remarkably, the non-interacting model of the Fermi gas reproduces many qualitative features of metallic behavior, such as a well-defined Fermi surface, a linear specific heat capacity, and a temperature-independent paramagnetic susceptibility. Such "Landau Fermi liquid behavior" appears in many contexts - in metals at low temperatures, in the core of neutron stars, in liquid Helium-3 and most recently, it has become possible to create Fermi liquids with tunable interactions in atom traps. As we shall see, our understanding of Landau Fermi liquids is intimately linked with the idea of adiabaticity introduced in the last chapter.

In the 1950's, physicists on both sides of the Iron curtain pondered the curious robustness of Fermi liquid physics against interactions. In Princeton New Jersey, David Bohm and David Pines, carried out the first quantization of the interacting electron fluid, proposing that the effects of long-range interactions are absorbed by a canonical transformation that separates the excitations into a high frequency plasmon and a low frequency fluid of renormalized electrons[**?**]. On the other side of the world, Lev Landau at the Kapitza Low Temperature Institute in Moscow, came to the conclusion that the robustness of the Fermi liquid is linked with the idea of adiabaticity and the Fermi exclusion principle[**?**].

At first sight, the possibility that an almost free Fermi fluid might survive the effect of interactions seems hopeless. With interactions, a moving fermion decays by emitting arbitrary numbers of low-energy particle-hole pairs, so how can it ever form a stable particle-like excitation? Landau realized that a fermion outside the Fermi surface can not scatter into an occupied momentum state below the Fermi surface, so the closer it is to the Fermi surface, the smaller the phase space available for decay. We will see that as a consequence, the inelastic scattering rate grows quadratically with excitation energy ϵ and temperature

$$\tau^{-1}(\epsilon) \propto (\epsilon^2 + \pi^2 T^2).$$

In this way, particles at the Fermi energy develop an infinite lifetime. Landau named these long-

lived excitations "quasi-particles". "Landau Fermi liquid theory"[**? ? ? ?**] describes the collective physics of a fluid of these quasiparticles.

It was a set of experiments on liquid Helium-3 (^3He), half a world away from Moscow, that helped to crystallize Landau's ideas. In the aftermath of the Second World War, the availability of isotopically pure ^3He as a byproduct of the Manhattan project, made it possible, for the first time, to experimentally study this model Fermi liquid. The first measurements were carried at Duke University in North Carolina, by Fairbank, Ard and Walters. [**?**]. While Helium-4 atoms are bosons, atoms of the much rarer isotope, $He-3$ are spin-1/2 fermions. These atoms contain a neutron and two protons in the nucleus, neutralized by two orbital electrons in a singlet state, forming a composite, neutral fermion. ^3He is a much much simpler quantum fluid than the electron fluid of metals:

- without a crystal lattice, liquid ^3He is isotropic and enjoys the full translational and Gallilean symmetries of the vacuum.
- ^3He atoms are neutral, interacting via short-range interactions, avoiding the complications of a long-range Coulomb interaction in metals.

Prior to Landau's theory, the only available theory of a degenerate Fermi liquid was Sommerfeld's model for non-interacting Fermions. A key property of the non-interacting Fermi-liquid, is the presence of a large, finite density of single-particle excitations at the Fermi energy, given by [1]

$$N(0) = 2\frac{(4\pi)p^2}{(2\pi\hbar)^3}\frac{dp}{d\epsilon_p}\bigg|_{p=p_F} = \frac{mp_F}{\pi^2\hbar^3}. \tag{7.1}$$

The argument of $N(\epsilon)$ is the energy $\epsilon = E - \mu$ measured relative to the chemical potential, μ. The density of states per unit volume, per spin is $N(0)/2$. A magnetic field splits the "up" and "down" Fermi surfaces, shifting their energy by an amount $-\sigma\mu_F B$, where $\sigma = \pm 1$ and $\mu_F = \frac{g}{2}\frac{e\hbar}{2m}$ is half the product of the Bohr magneton for the fermion and the g-factor associated with its spin. The number of "up" and "down fermions is thereby changed by an amount $\delta N_\uparrow = -\delta N_\downarrow = \frac{1}{2}N(0)(\mu_F B)$, inducing a net magnetization $M = \chi B$ where,

$$\chi = \mu_F(N_\uparrow - N_\downarrow)/B = \mu_F^2 N(0) \tag{7.2}$$

is the "Pauli paramagnetic susceptibility". For electrons, $g \approx 2$ and $\mu_F \equiv \mu_B = \frac{e\hbar}{2m}$ is the Bohr magneton, so the Pauli susceptibility of a free electron gas is $\mu_B^2 N(0)$.

In a degenerate Fermi liquid, the energy is given by

$$\mathcal{E}(T) = E(T) - \mu N = \sum_{\mathbf{k}\sigma=\pm\mathbf{1}/\mathbf{2}} \epsilon_{\mathbf{k}} \frac{1}{e^{\beta\epsilon_{\mathbf{k}}} + 1} \tag{7.3}$$

Here, we use the notation $\mathcal{E} = E - \mu N$ to denote the energy measured in the grand-canonical ensemble. The variation of this quantity at low temperatures (where to order T^2, the chemical

[1] **Note**: In the discussion that follows, we shall normalize all extensive properties per unit volume, thus the density of states, $N(\epsilon)$ the specific heat C_V, or the magnetization M, will all refer to those quantities, per unit volume.

potential is constant) depends only on the free-particle density of states at the Fermi energy, $N(0)$. The low temperature specific heat

$$\begin{aligned} C_V &= \frac{d\mathcal{E}}{dT} = N(0)\int_{-\infty}^{\infty} d\epsilon\epsilon\frac{d}{dT}\left(\frac{1}{e^{\beta\epsilon}+1}\right) \\ &= N(0)k_B^2 T\overbrace{\int_{-\infty}^{\infty} dx\frac{x^2}{(e^x+1)(e^{-x}+1)}}^{\pi^2/3} = \overbrace{\frac{\pi^2}{3}N(0)k_B^2}^{=\gamma} T \end{aligned} \tag{7.4}$$

is linear in temperature. Since both the specific heat, and the magnetic susceptibility are proportional to the density of states, the ratio of these two quantities $W = \chi/\gamma$, often called the Wilson ratio or "Stoner enhancement factor", is set purely by the size of the magnetic moment:

$$W = \frac{\chi}{\gamma} = 3\left(\frac{\mu_F}{\pi k_B}\right)^2 \tag{7.5}$$

Fairbank, Ard and Walters' experiment confirmed the Pauli paramagnetism of liquid in Helium-3, but the measured Wilson ratio is about ten times larger than predicted by Sommerfeld theory. Landau's explanation of these results is based on the idea that one can track the evolution of the properties of the Fermi liquid by adiabatically switching on the interactions. He considered a hypothetical gas of non-interacting Helium atoms with no forces of repulsion between for which Sommerfeld's model would certainly hold. Suppose the interactions are now turned on slowly. Landau argued that since the fermions near the Fermi surface had nowhere to scatter to, the low-lying excitations of the Fermi liquid would evolve adiabatically, in the sense discussed in the last chapter, so that that each quantum state of the fully-interacting liquid Helium-3, would be in *precise one-to-one correspondence with the states of the idealized "non-interacting" Fermi-liquid*.[**?**]

7.2 The Quasiparticle Concept

The "quasiparticle" concept is a triumph of Landau's Fermi liquid theory, for it enables us to continue using the idea of an independent particle, even in the presence of strong interactions; it also provides a framework for understanding the robustness of the Fermi surface while accounting for the effects of interactions.

A quasiparticle is the adiabatic evolution of the non-interacting fermion into an interacting environment. The conserved quantum numbers of this excitation: its spin and its "charge" and its momentum are unchanged but Landau reasoned that that its dynamical properties, the effective magnetic moment and mass of the quasiparticle would be " renormalized" to new values g^* and m^* respectively. Subsequent measurements on ^3He[**? ?**] revealed that the quasiparticle mass and enhanced magnetic moment g^* are approximately

$$\begin{aligned} m^* &= (2.8)m_{(He^3)}, \\ (g^*)^2 &= 3.3(g^2)_{(He^3)}. \end{aligned} \tag{7.6}$$

These "renormalizations" of the quasiparticle mass and magnetic moment are elegantly accounted for in Landau Fermi liquid theory in terms of a small set of "Landau parameters" which characterize the interaction, as we now shall see.

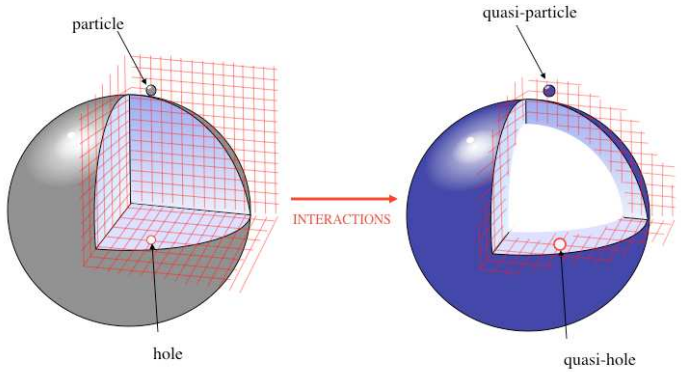


Figure 7.1: In the non-interacting Fermi liquid (a), a stable particle can be created anywhere outside the Fermi surface, a stable hole excitation anywhere inside the Fermi surface. (b) When the interactions are turned on adiabatically, particle excitations near the Fermi surface adiabatically evolve into "quasiparticles", with the same charge, spin and momentum. Quasiparticles and quasi-holes are only well defined near the Fermi surface of the Landau Fermi Liquid.

Let us label the momentum of each particle in the original non-interacting Fermi liquid by $\tilde{\mathrm{p}}$ and spin component $\sigma = \pm 1/2$. The number of fermions momentum $\vec{p}$, spin component σ, $n_{\mathrm{p}\sigma}$, is either one, or zero. The complete quantum state of the non-interacting system is labeled by these occupancies. We write

$$\Psi = |n_{\mathrm{p}_1\sigma_1},\, n_{\mathrm{p}_2\sigma_2}, \ldots\rangle \tag{7.7}$$

In the ground-state, Ψ_o all states with momentum p less than the Fermi momentum are occupied, all states above the Fermi surface are empty

$$\text{Ground} - \text{state } \Psi_{\mathrm{o}} \quad : \quad n_{\mathrm{p}\sigma} = \begin{cases} 1 & (\mathrm{p} < \mathrm{p_F}) \\ 0 & (\text{otherwise } \mathrm{p} > \mathrm{p_F}) \end{cases} \tag{7.8}$$

Landau argued, that if one turned on the interactions infinitely slowly, then this state would evolve smoothly into the ground-state of the interacting Fermi liquid. This is an example of the adiabatic evolution encountered in the previous chapter. For the adiabatic evolution to work, the Fermi liquid ground-state has to remain stable. This is a condition that certainly fails when the system undergoes a phase transition into another ground-state, a situation that may occur at a certain critical interaction strength. However, up to this critical value, the adiabatic evolution of the ground-state can take place. The energy of the final ground-state is unknown, but we can call it E_0.

Suppose we now add a fermion above the Fermi surface of the original state. We can repeat the the adiabatic switch-on of the interactions, but it is a delicate procedure for an excited state, because away from the Fermi surface, an electron can decay by emitting low-energy particle-hole pairs which disipates its energy in an irreversible fashion. To avoid this irreversibility, the lifetime of the particle τ_e must be longer than the adiabatic "switch-on" time $\tau_A = \epsilon^{-1}$ encountered in (6.87), and since this time becomes infinite, strict adiabaticity is only possible for excitations that lie on the Fermi surface, where τ_e is infinite. A practical Landau Fermi liquid theory requires that we consider excitations that are a finite distance away from the Fermi surface, and when we do this, we tacitly ignore the finite lifetime of the quasiparticles. By doing so, we introduce an error of order $\tau_e^{-1}/\epsilon_{\mathbf{p}}$. This error can be made arbitrarily small, provided we restrict our attention to small perturbations to the ground-state.

Adiabatic evolution conserves the momentum of the quasiparticle state, which will then evolve smoothly into a final state that we can label as:

$$\text{Quasi}-\text{particle}: \ \Psi_{\mathbf{p}_o\sigma_o} \qquad n_{\mathrm{p}\sigma} = \begin{cases} 1 & (\mathrm{p} < \mathrm{p_F} \text{ and } \mathbf{p} = \mathbf{p}_o, \sigma = \sigma_o) \\ 0 & (\text{otherwise}) \end{cases} \tag{7.9}$$

This state has total momentum $\mathbf{p}_o$ where $|\mathbf{p}_o| > p_F$ and an energy $E(\mathrm{p_o}) > E_o$ larger than the ground-state. It is called a "quasiparticle-state" because it behaves in almost every respect like a single particle. Notice in particular, that the the Fermi surface momentum p_F is preserved by the adiabatic introduction of interactions. Unlike free particles however, the Landau quasiparticle is only a well-defined concept close to the Fermi surface. Far from the Fermi surface, quasiparticles develop a lifetime, and once the lifetime is comparable with the quasiparticle excitation energy, the quasiparticle concept loses its meaning.

The energy required to create a single quasiparticle, is

$$E^{(0)}_{\mathrm{p_o}} = E(p_o) - E_o \tag{7.10}$$

where the superscript (0) denotes a single excitation in the absence of any other quasiparticles. We shall mainly work in the Grand canonical ensemble, using $\mathcal{E} = E - \mu N$ in place of the absolute energy, where μ is the chemical potential, enabling us to explore the variation of the energy at constant particle number N. The corresponding quasiparticle excitation energy is then

$$\epsilon^{(0)}_{\mathrm{p_o}} = E^{(0)}_{\mathrm{p_o}} - \mu = \mathcal{E}(p_o) - \mathcal{E}_o. \tag{7.11}$$

Notice, that since $|\mathbf{p}_0| > p_F$, this energy is positive.

In a similar way, we can also define a "quasi-hole" state, in which a quasiparticle is removed the Fermi sea,

$$\text{Quasi}-\text{hole}: \ \overline{\Psi}_{\mathrm{p_o}\sigma_o} \qquad n_{\mathrm{p}\sigma} = \begin{cases} 1 & (\mathrm{p} < \mathrm{p_F} \textit{ except when } \mathbf{p} = \mathbf{p}_o, \sigma = \sigma_o) \\ 0 & (\text{otherwise}) \end{cases}, \tag{7.12}$$

where the bar is used to denote the hole and now, $|\mathbf{p}_o| < p_F$ is beneath the Fermi surface. The energy of this state is $\overline{E}(\mathbf{p}_o) = E_o - E_{\mathbf{p}_0}$, since we have removed a particle. Now the change in particle number is $\Delta N = -1$, so the the excitation energy of a single quasi-hole, measured in the Grand Canonical ensemble, is then

$$\overline{\epsilon}^{(0)}_{\mathbf{p}_o} = -E^{(0)}_{\mathbf{p}_o} + \mu = -\epsilon^{(0)}_{\mathbf{p}_o}, \tag{7.13}$$

i.e the energy to create a quasihole is the negative of the corresponding quasiparticle energy $\epsilon_{\mathbf{p}_o}$. Of course, when $|\mathbf{p}_o| < p_F$, $\epsilon_{\mathbf{p}_o} < 0$ so that the quasihole excitation energy $\overline{\epsilon^{(0)}}_{\mathbf{p}_o}$ is always positive, as required for a stable ground-state. In this way, the energy to create a quasihole, or quasiparticle is always given by $|\epsilon_{\mathbf{p}_o}|$, independently of whether $\mathbf{p}_o$ is above, or below the Fermi surface.

The quasiparticle concept would be of limited value if it was limited to individual excitations. At a finite temperature, a dilute gas of these particles is excited around the Fermi surface and these particles interact. How can the particle concept survive once one has a finite density of excitations? Landau's appreciation of a very subtle point enabled him to answer this question. He realized that the amount of momentum that two particles can exchange in a collision while satisfying the exclusion principle goes to zero for particles that are on the Fermi surface:

$$(\mathbf{p}_1, \mathbf{p}_2) \to (\mathbf{p}_1 - \mathbf{q}, \mathbf{p}_2 + \mathbf{q}) \qquad (\mathbf{q} = 0 \text{ on Fermi surface.}) \tag{7.14}$$

On the Fermi surface, particles *only* scatter in the *forward direction*, so in the low-energy limit, the number of particles at a given momentum is becomes a constant of the motion. In this way, the Landau Fermi liquid is characterized by an *infinite* set of conserved quantities $n_{\mathbf{p}\sigma}$, so that on the Fermi surface,

$$[H, n_{\mathbf{k}\sigma}] = 0. \qquad (\mathbf{p} \in \mathrm{FS}) \tag{7.15}$$

The challenge is to develop a theory that describes the Free energy $F[\{n_{\mathbf{p}\sigma}\}$ and the slow long distance hydrodynamics of these conserved quantities.

Example 7.1: Suppose $|\Psi_0\rangle = \prod_{|\mathbf{p}|<p_F,\sigma} c^\dagger_{\mathbf{p}\sigma}|0\rangle$ is the ground-state of a non-interacting Fermi liquid, where $c^\dagger_{\mathbf{p}\sigma}$ creates a "bare" fermion. By considering the process of adiabatically turning on the interaction, time-evolving the one-particle state $c^\dagger_{\mathbf{p}_o\sigma}|FS\rangle$ from the distant past to the present ($t = 0$) in the interaction representation, write down an expression for the ground-state wavefunction $|\psi\rangle$ and the quasiparticle creation operator of the fully interacting system.

Solution: The time-evolution operator from the distant past in the interaction representation is

$$U = T \exp\left[-i \int_{-\infty}^{0} \hat{V}_I(t) dt\right]$$

where $\hat{V}_I(t)$ is the interaction operator, written in the interaction representation. If we add a particle to the filled Fermi sea, and adiabatically time evolve from the distant past to the present, we obtain

$$c^\dagger_{\mathbf{p}\sigma}|\Psi_0\rangle \longrightarrow Uc^\dagger_{\mathbf{p}\sigma}|\Psi_0\rangle = \overbrace{(Uc^\dagger_{\mathbf{p}\sigma}U^\dagger)}^{QPa^\dagger_{\mathbf{p}\sigma}}\overbrace{U|\Psi_0\rangle}^{|\phi\rangle}.$$

If the adiabatic evolution avoids a quantum phase transition, then

$$|\phi\rangle = U|FS\rangle$$

is the ground-state of the fully interacting system. In this case, we may interpret

$$a^\dagger_{\mathbf{p}\sigma} = (Uc^\dagger_{\mathbf{p}\sigma}U^\dagger)$$

as the "quasiparticle creation operator". Note that if we try to rewrite this object in terms of the original creation operator, $c^\dagger_{\mathbf{p}\sigma}$, it involves combinations of one fermion with particle-hole pairs. See section 7.8 for a more detailed discussion.

7.3 The Neutral Fermi liquid

These physical considerations led Landau to conclude that the energy of a gas of quasiparticles could be expressed as a functional of the quasiparticles occupancies $n_{\mathbf{p}\sigma}$. Following Landau, we shall develop the Fermi liquid concept using an idealized "neutral" Landau Fermi liquid, like $He-3$, in which the quasiparticles move in free space, interacting isotropically via a short range interaction, forming a neutral fluid.

If the density of quasiparticles is low, it is sufficient to expand the energy in the small deviations in particle number $\delta n_{\mathbf{p}\sigma} = n_{\mathbf{p}\sigma} - n^{(o)}_{\mathbf{p}\sigma}$ from equilibrium. This leads to the Landau energy functional $\mathcal{E}(\{n_{\mathbf{p}\sigma}\}) = E(\{n_{\mathbf{p}\sigma}\}) - \mu N$, where

$$\mathcal{E} = \mathcal{E}_0 + \sum_{\mathbf{p}\sigma}(E^{(0)}_{\mathbf{p}\sigma} - \mu)\delta n_{\mathbf{p}\sigma} + \frac{1}{2}\sum_{\mathbf{p},\mathbf{p}',\sigma,\sigma'} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\delta n_{\mathbf{p}\sigma}\delta n_{\mathbf{p}'\sigma'} + \ldots. \tag{7.16}$$

The first order coefficient

$$\epsilon^{(0)}_{\mathbf{p}\sigma} \equiv E^{(0)}_{\mathbf{p}\sigma} - \mu = \frac{\delta\mathcal{E}}{\delta n_{\mathbf{p}\sigma}} \tag{7.17}$$

describes the excitation energy of an isolated quasiparticle. Provided we can ignore spin-orbit interactions, then the total magnetic moment is a conserved quantity, so the magnetic moments of the quasiparticles are preserved by interactions. In this case, $\epsilon^{(0)}_{\mathbf{p}\sigma} = \epsilon^{(0)}_{\mathbf{p}} - \sigma\mu_F B$, where μ_F is the un-renormalized magnetic moment of an isolated fermion.

The quasiparticle energy can be expanded linearly in momentum near the Fermi surface

$$E^{(0)}_p = v_F(p - p_F) + \mu^{(0)}, \tag{7.18}$$

where v_F is the Fermi velocity at the Fermi energy $\mu^{(0)}$, where μ^0 is the chemical potential in the ground-state. The quasiparticle effective mass m^* is then defined in terms of v_F as

$$v_F = \left.\frac{d\epsilon^{(0)}_p}{dp}\right|_{p=p_F} = \frac{p_F}{m^*}. \tag{7.19}$$

We can use this mass to define a quasiparticle density of states

$$N^*(\epsilon) = 2\sum_{\mathbf{p}}\delta(\epsilon - \epsilon^{(0)}_{\mathbf{p}}) = 2\int\frac{4\pi p^2 dp}{(2\pi\hbar)^3}\delta(\epsilon - \epsilon^{(0)}_p) = \frac{p^2}{\pi^2\hbar^3}\frac{dp}{d\epsilon^0_p}. \tag{7.20}$$

Using (7.19), it follows that

$$N^*(0) = \frac{m^* p_F}{\pi^2\hbar^3}. \tag{7.21}$$

In this way, the effective mass m^* determines the density of states at the Fermi energy: large effective masses lead to large densities of states.

The second-order coefficients

$$f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'} = \left.\frac{\delta^2\mathcal{E}}{\delta n_{\mathbf{p}\sigma}\delta n_{\mathbf{p}'\sigma'}}\right|_{\delta n_{\mathbf{p}''\sigma''}=0} \tag{7.22}$$

describe the interactions between quasiparticles at the Fermi surface. These partial derivatives are evaluated in the presence of an otherwise *"frozen" Fermi sea*, where all other quasiparticle occupancies are fixed. Landau was able to show that in an isotropic Fermi liquid, the quasiparticle mass m^* is related to the dipolar component of these interactions, as we shall shortly demonstrate. The Landau interaction can be regarded as an interaction operator that acts on a the thin shell of quasiparticle states near the Fermi surface. If $\hat{n}_{\mathbf{p}\sigma} = \psi^\dagger_{\mathbf{p}\sigma}\psi_{\mathbf{p}\sigma}$ is the quasiparticle occupancy, where $\psi^\dagger_{\mathbf{p}\sigma}$ is the quasiparticle creation operator, then one is tempted to write

$$H_I \sim \frac{1}{2}\sum_{\mathbf{p}\sigma\mathbf{p}'\sigma'} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\hat{n}_{\mathbf{p}\sigma}\hat{n}_{\mathbf{p}'\sigma'}.$$

Written this way, we see that the Landau interaction term is a *"forward scattering amplitude"* between quasiparticles whose initial and final momenta are unchanged. In practice, one has to allow for slowly varying quasiparticle densities, $n_{\mathbf{p}\sigma}(\mathbf{x})$, writing

$$H_I \sim \frac{1}{2}\int d^3x\sum_{\mathbf{p}\sigma\mathbf{p}'\sigma'} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\hat{n}_{\mathbf{p}\sigma}(\mathbf{x})\hat{n}_{\mathbf{p}'\sigma'}(\mathbf{x}).$$

where $n_{\mathbf{p}\sigma}(\mathbf{x})$ is the local quasiparticle density. Using the Fourier transformed density operator $\hat{n}_{\mathbf{p}\sigma}(\mathbf{q}) = \psi^\dagger_{\mathbf{p}-\mathbf{q}/2\sigma}\psi_{\mathbf{p}+\mathbf{q}/2\sigma} = \int_{\mathbf{x}} e^{-i\mathbf{q}\cdot\mathbf{x}}n_{\mathbf{p}\sigma}(\mathbf{x})$, a more correct formulation of the Landau interaction is

$$H_I = \frac{1}{2}\sum_{\mathbf{p}\sigma\mathbf{p}'\sigma',|\mathbf{q}|<\Lambda} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}(\mathbf{q})\hat{n}_{\mathbf{p}\sigma}(\mathbf{q})\hat{n}_{\mathbf{p}'\sigma'}(-\mathbf{q}). \tag{7.23}$$

where Λ is a cutoff that restricts the momentum transfer to values smaller than the thickness of the shell of quasiparticles. The Landau coefficients for the neutral Fermi liquid are then the zero momentum limit $f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'} = f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}(\mathbf{q}=0)$. The existence of such a limit requires that the interaction has a finite range, so that the its Fourier transform at $\mathbf{q}=0$ is well-defined. This requirement is met in neutral Fermi liquids, however the Coulomb interaction does not meet this requirement. The extension of Landau's Fermi liquid concept to charged Fermi liquids requires that we separate out the long-range part of the Coulomb interaction - a point that will be returned to later.

Interactions mean that quasiparticle energies are sensitive to changes in the quasiparticle occupancies. Suppose the quasiparticle occupancies deviate from the ground-state as follows $n_{\mathbf{p}\sigma} \to n_{\mathbf{p}\sigma} + \delta n_{\mathbf{p}\sigma}$. The corresponding change in the total energy is then

$$\frac{\delta \mathcal{E}}{\delta n_{\mathbf{p}\sigma}} = \epsilon_{\mathbf{p}\sigma} \equiv E_{\mathbf{p}\sigma} - \mu = \epsilon^{(0)}_{\mathbf{p}\sigma} + \sum_{\mathbf{p}'\sigma'} f_{\mathbf{p}\sigma,\mathbf{p}',\sigma'}\delta n_{\mathbf{p}'\sigma'}. \tag{7.24}$$

The second-term is change in the quasiparticle energy induced by the polarization of the Fermi sea.

To determine thermodynamic properties of the Landau Fermi liquid we also need to know the entropy of the fluid. Fortunately, when we turn on interactions adiabatically, the entropy is invariant, so that it must maintain the dependence on particle occupancies that it has in the non-interacting system, i.e.

$$S = -k_B \sum_{\mathbf{p},\sigma} [n_{\mathbf{p}\sigma}\ln n_{\mathbf{p}\sigma} + (1-n_{\mathbf{p}\sigma})\ln(1-n_{\mathbf{p}\sigma})] \tag{7.25}$$

The full thermodynamics are determined by the the Free energy $F = \mathcal{E} - TS = E - \mu N - TS$, which is the sum of (7.16) and (7.25).

$$\begin{aligned} F(\{n_{\mathbf{p}\sigma}\}) &= \mathcal{E}_0(\mu) + \sum_{\mathbf{p}\sigma} \epsilon^{(0)}_{\mathbf{p}\sigma}\delta n_{\mathbf{p}\sigma} + \frac{1}{2}\sum_{\mathbf{p},\mathbf{p}',\sigma,\sigma'} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\delta n_{\mathbf{p}\sigma}\delta n_{\mathbf{p}'\sigma'} \\ &+ k_B T \sum_{\mathbf{p},\sigma} [n_{\mathbf{p}\sigma}\ln n_{\mathbf{p}\sigma} + (1-n_{\mathbf{p}\sigma})\ln(1-n_{\mathbf{p}\sigma})] \end{aligned} \tag{7.26}$$

Free energy of Landau Fermi Liquid.

Table. 8.1 Key Properties of the Fermi Liquid .

PROPERTY	NON-INTERACTING	LANDAU FERMI LIQUID
Fermi momentum	p_F	unchanged
Density of particles	$2\frac{V_{FS}}{(2\pi)^3}$	unchanged
Density of states	$N(0) = \frac{mp_F}{\pi^2\hbar^3}$	$N^*(0) = \frac{m^*p_F}{\pi^2\hbar^3}$
Effective mass	m	$m^* = m(1+F_1^s)$
Specific heat Coefficient $C_V = \gamma T$	$\gamma = \frac{\pi^2}{3}k_B^2 N(0)$	$\gamma = \frac{\pi^2}{3}k_B^2 N^*(0)$
Spin susceptibility	$\chi_s = \mu_F^2 N(0)$	$\chi_s = \mu_F^2 \frac{N^*(0)}{1+F_0^a}$
Charge Susceptibility	$\chi_C = N(0)$	$\chi_C = \frac{N^*(0)}{1+F_0^s}$
Collective modes	-	Sound ($\omega\tau << 1$) Zero sound ($\omega\tau >> 1$)

Table 8.1 summarizes the key properties of the Landau Fermi liquid.

7.3.1 Landau Parameters

The power of the Landau Fermi liquid theory lies in its ability to parameterize the interactions in terms of a small number of multipole parameters called "Landau Parameters". These parameters describe how the original non-interacting Fermi liquid theory is renormalized by the feedback effect of interactions on quasiparticle energies.

In a Landau Fermi liquid in which spin is conserved, the interaction is invariant under spin

rotations and can in general be written in the form [2]

$$f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'} = f^s_{\mathbf{p},\mathbf{p}'} + f^a_{\mathbf{p},\mathbf{p}'}\sigma\sigma'. \tag{7.27}$$

The spin-dependent part of the interaction is the magnetic component of the quasiparticle interaction.

In practice, we are only interested in quasiparticles with a small excitation energy, so we only need to know the values of $f^{s,a}_{\mathbf{p},\mathbf{p}'}$ near the Fermi surface, permitting us to set $\mathbf{p} = p_F\hat{\mathbf{p}}$, $\mathbf{p}' = p_F\hat{\mathbf{p}}'$, where $\hat{\mathbf{p}}$ and $\hat{\mathbf{p}}'$ are the unit vectors on the Fermi surface. In an isotropic Landau Fermi liquid, the physics is invariant under spatial rotations, so that interactions on the Fermi surface only depend on the relative angle θ between $\hat{\mathbf{p}}$ and $\hat{\mathbf{p}}'$. We write

$$f^{s,a}_{\mathbf{p},\mathbf{p}'} = f^{s,a}(\cos\theta), \qquad (\cos\theta = \hat{\mathbf{p}}\cdot\hat{\mathbf{p}}'). \tag{7.28}$$

We convert the interaction to a dimensionless function by multiplying it with the quasiparticle density of states $N^*(0)$:

$$F^{s,a}(\cos\theta) = N^*(0)f^{s,a}(\cos\theta) \tag{7.29}$$

These functions can now be expanded as a multipole expansion in terms of Legendre polynomials

$$F^{s,a}(\cos\theta) = \sum_{l=0}^{\infty}(2l+1)F^{s,a}_l P_l(\cos\theta). \tag{7.30}$$

The coefficients F^s_l and F^a_l are the Landau parameters. The spin-symmetric components F^s_l parameterize the non-magnetic part of the interaction while the spin-antisymmetric F^a_l define the magnetic component of the interaction. These parameters determine how distortions of the the Fermi surface are fed-back to modify quasiparticle energies.

We can invert (7.30) using the orthogonality relation $\frac{1}{2}\int_{-1}^{1} dc\; P_l(c)P_{l'}(c) = (2l+1)^{-1}\delta_{l,l'}$,

$$F^{s,a}_l = \tfrac{1}{2}\int_{-1}^{1} dc\; F^{s,a}(c)P_l(c) \equiv \langle F^{s,a}(\hat{\Omega})P_l(\hat{\Omega})\rangle_{\hat{\Omega}}, \tag{7.31}$$

where $\langle\ldots\rangle_{\hat{\Omega}}$ denotes an average over solid angle. It is useful to rewrite this angular average as an average over the Fermi surface. To do this we note that since $2\sum_{\mathbf{k}}\delta(\epsilon_{\mathbf{k}}) = N^*(0)$, the function $\frac{2}{N^*(0)}\delta(\epsilon_{\mathbf{k}})$ behaves as a normalized "projector" onto the Fermi surface, so that

$$F^{s,a}_l = \langle F^{s,a}(\hat{\Omega})P_l(\hat{\Omega})\rangle_{FS} = \frac{2}{N^*(0)}\sum_{\mathbf{p}'} F^{s,a}_{\mathbf{p},\mathbf{p}'}P_l(\cos\theta_{\mathbf{p},\mathbf{p}'})\delta(\epsilon_{\mathbf{p}'}), \tag{7.32}$$

[2] To see that this result follows from spin rotation invariance, we need to recognize that the quasiparticle occupancies $n_{\mathbf{p}\sigma}$ we have considered are actually the diagonal elements of a quasiparticle density matrix $n_{\mathbf{p}\alpha\beta}$. With this modification, the interaction becomes a matrix $f_{\mathbf{p}\alpha\beta;\mathbf{p}'\gamma\eta}$ whose most general rotationally invariant form is

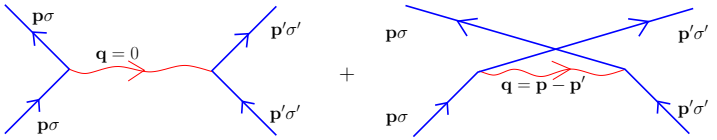
$$f_{\mathbf{p}\alpha\beta;\mathbf{p}'\gamma\eta} = f^s(\mathbf{p},\mathbf{p}')\delta_{\alpha\beta}\delta_{\gamma\eta} + f^a(\mathbf{p},\mathbf{p}')\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\gamma\eta}.$$

The diagonal components of this interaction recover the results of (7.27)

and since $F^{s,a}_{\mathbf{p},\mathbf{p}'} = N^*(0)f^{s,a}_{\mathbf{p},\mathbf{p}'}$,

$$F^{s,a}_l = 2\sum_{\mathbf{p}'} f^{s,a}_{\mathbf{p},\mathbf{p}'}P_l(\cos\theta_{\mathbf{p},\mathbf{p}'})\delta(\epsilon_{\mathbf{p}'}). \tag{7.33}$$

This form is very convenient for later calculations.



$V(\mathbf{q}=0)$ $\qquad -V(\mathbf{p}-\mathbf{p}')\delta_{\sigma\sigma'}$

$$f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'} = V(\mathbf{q}=0) - V(\mathbf{p}-\mathbf{p}')\delta_{\sigma\sigma'}$$

Figure 7.2: Feynman diagrams for leading order contributions to the Landau parameter for an interaction $V(\mathbf{q})$. Wavy line represents the interaction between quasiparticles.

Example 7.2: Use first order perturbation theory to calculate the Landau interaction parameters for a fluid of fermions with a weak interaction described by

$$H = \sum_{\mathbf{p}\sigma} E_{\mathbf{p}}n_{\mathbf{p}\sigma} + \frac{\lambda}{2}\sum_{\mathbf{p}\sigma,\mathbf{p}'\sigma',\mathbf{q}} V(q)c^\dagger_{\mathbf{p}-\mathbf{q}\sigma}c^\dagger_{\mathbf{p}'+\mathbf{q}\sigma'}c_{\mathbf{p}'\sigma'}c_{\mathbf{p}\sigma}$$

where $E_{\mathbf{p}}$ is the energy of the non-interacting Fermi gas, $V(q) = \int \frac{d^3q}{(2\pi)^3}e^{-i\mathbf{q}\cdot\mathbf{r}}V(r)$ is the Fourier transform of the interaction potential $V(r)$ and $\lambda << 1$ is a very small coupling constant. Hint: use first order perturbation theory in λ to compute the energy of a state

$$\Psi = |n_{\mathbf{p}_1\sigma_1},\; n_{\mathbf{p}_2\sigma_2},\ldots\rangle$$

to leading order in the interaction strength λ, and then read off the terms quadratic in $n_{\mathbf{p}\sigma}$.
Solution:

To leading order in λ, the total energy is given by $E = \langle\Psi|H|\Psi\rangle$, or

$$E = \sum_{\mathbf{p}\sigma} E_{\mathbf{p}}n_{\mathbf{p}\sigma} + \frac{\lambda}{2}\sum_{\mathbf{p}\sigma,\mathbf{p}'\sigma',\mathbf{q}} V(q)\langle\Psi|c^\dagger_{\mathbf{p}-\mathbf{q}\sigma}c^\dagger_{\mathbf{p}'+\mathbf{q}\sigma'}c_{\mathbf{p}'\sigma'}c_{\mathbf{p}\sigma}|\Psi\rangle. \tag{7.34}$$

The matrix element $\langle\Psi|c^\dagger_{\mathbf{p}-\mathbf{q}\sigma}c^\dagger_{\mathbf{p}'+\mathbf{q}\sigma'}c_{\mathbf{p}'\sigma'}c_{\mathbf{p}\sigma}|\Psi\rangle$ in the interaction term vanishes unless the two quasiparticle state annihilated by the two destruction operators has an overlap with the two particle state created by the two creation operators, i.e.

$$\langle\Psi|c^\dagger_{\mathbf{p}-\mathbf{q}\sigma}c^\dagger_{\mathbf{p}'+\mathbf{q}\sigma'}c_{\mathbf{p}'\sigma'}c_{\mathbf{p}\sigma}|\Psi\rangle \quad = \quad \langle\mathbf{p}-\mathbf{q},\sigma;\mathbf{p}'+\mathbf{q},\sigma'|\mathbf{p},\sigma;\mathbf{p}'\sigma'\rangle n_{\mathbf{p}\sigma}n_{\mathbf{p}\sigma'}$$

$$= \left(\delta_{\mathbf{q}=0} - \delta_{\mathbf{p}-\mathbf{q},\mathbf{p}'}\delta_{\sigma,\sigma'}\right) n_{\mathbf{p}\sigma} n_{\mathbf{p}\sigma'} \tag{7.35}$$

where the second term occurs when the outgoing state is the "exchange" of the incoming two-quasiparticle state.

Inserting (7.35) into (7.34), we obtain

$$\sum_{\mathbf{p}\sigma} E_{\mathbf{p}} n_{\mathbf{p}\sigma} + \frac{\lambda}{2} \sum_{\mathbf{p}\sigma,\mathbf{p}'\sigma'} [V(0) - V(\mathbf{p}-\mathbf{p}')\delta_{\sigma\sigma'}] n_{\mathbf{p}'\sigma'} n_{\mathbf{p}\sigma}$$

enabling us to read off the Landau interaction as

$$f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'} = \lambda[V(q=0) - V(\mathbf{p}-\mathbf{p}')\delta_{\sigma\sigma'}] + O(\lambda^2).$$

It follows that the symmetric and antisymmetric parts of the interaction parameters are

$$\begin{aligned} f^s_{\mathbf{p},\mathbf{p}'} &= \lambda[V(q=0) - \frac{1}{2}V(\mathbf{p}-\mathbf{p}')] + O(\lambda^2) \\ f^a_{\mathbf{p},\mathbf{p}'} &= -\frac{\lambda}{2}V(\mathbf{p}-\mathbf{p}') + O(\lambda^2). \end{aligned} \tag{7.36}$$

Note that

- The Landau interaction is only well-defined if $V(q=0)$ is finite, which implies that the interaction is short-ranged.
- The second term in the interaction corresponds to the "exchange" of identical particles. For a repulsive interaction, this gives rise to an *attractive* f^a. We can represent the interaction term by the Feynman diagrams shown in (***).

7.3.2 Equilibrium distribution of quasiparticles

Remarkably, despite interactions, the Landau Fermi liquid preserves the equilibrium Fermi-Dirac momentum distribution. The key idea here is that in thermal equilibrium, the free energy (7.26) is stationary with respect to small changes $\delta n_{\mathbf{p}\sigma}$ in quasiparticle occupancies, so that

$$\delta F = \sum_{\mathbf{p}\sigma} \delta n_{\mathbf{p}\sigma} \left[\epsilon_{\mathbf{p}\sigma} + k_B T \ln\left(\frac{n_{\mathbf{p}\sigma}}{1 - n_{\mathbf{p}\sigma}}\right)\right] + O(\delta {n_{\mathbf{p}\sigma}}^2) = 0. \tag{7.37}$$

Stationarity of the Free energy, $\delta F = 0$ enforces the thermodynamic identity $\delta F = \delta\mathcal{E} - T\delta S = 0$, or $d\mathcal{E} = TdS$. This requires that the linear coefficient of $\delta n_{\mathbf{p}\sigma}$ in (7.37) is zero, which implies that the quasiparticle occupancy

$$n_{\mathbf{p}\sigma} = \frac{1}{e^{\beta\epsilon_{\mathbf{p}\sigma}} + 1} = f(\epsilon_{\mathbf{p}\sigma}) \tag{7.38}$$

is determined by Fermi-Dirac distribution function of its energy. There is a subtlety here however, for the quantity $\epsilon_{\mathbf{p}\sigma}$ contains the feedback effect of interactions, as given in (7.24)

$$\epsilon_{\mathbf{p}\sigma} = \epsilon^{(0)}_{\mathbf{p}\sigma} + \sum_{\mathbf{p}'\sigma'} f_{\mathbf{p}\sigma,\mathbf{p}',\sigma'} \delta n_{\mathbf{p}'\sigma'}. \tag{7.39}$$

Let us first consider the low temperature behavior in the absence of a field. In this case, as the temperature is lowered, the density of thermally excited quasiparticles will go to zero, and in this limit, the quasiparticle distribution function is asymptotically given by

$$n_{\mathbf{p}\sigma} = f(\epsilon^{(0)}_{\mathbf{p}}).$$

In the ground-state this becomes a step function $n_{\mathbf{p}\sigma}|_{T=0} = \theta(-\epsilon^{(0)}_{\mathbf{p}}) = \theta(\mu - E^{(0)}_{\mathbf{p}})$, as expected.

To obtain the specific heat, we must calculate $C_V dT = d\mathcal{E} = \sum_{\mathbf{p}} \epsilon^{(0)}_{\mathbf{p}\sigma} \delta n_{\mathbf{p}\sigma}$. At low temperatures, $\delta n_{\mathbf{p}\sigma} = \frac{\partial f(\epsilon^{(0)}_{\mathbf{p}\sigma})}{\partial T} dT$, so that

$$C_V = \sum_{\mathbf{p}\sigma} \epsilon^{(0)}_{\mathbf{p}\sigma} \left(\frac{\partial f(\epsilon^{(0)}_{\mathbf{p}\sigma})}{\partial T}\right) \to N^*(0) \int_{-\infty}^{\infty} d\epsilon\, \epsilon \left(\frac{\partial f(\epsilon)}{\partial T}\right),$$

where, as in (7.4) the summation is replaced by an integral over the density of states near the Fermi surface. Apart from the renormalization of the energies, this is precisely the same result obtained in (7.4), leading to

$$C_V = \gamma T, \qquad \gamma = \frac{\pi^2 k_B^2}{3} N^*(0) \tag{7.40}$$

7.4 Feedback effects of interactions

One can visualize the Landau Fermi liquid as a deformable sphere, like a large water droplet in zero gravity. The Fermi sphere changes shape when the density or magnetization of the fluid is modified, or if a current flows. These deformations act back on the quasiparticles via the Landau interactions, to change the quasiparticle energies. These feedback effects are a generalization of the idea of a Weiss field in magnetism. When the feedback is positive, it can lead to instabilities, such as the development of magnetism. A Fermi surface can also oscillate collectively about its equilibrium shape. In a conventional gas, density oscillations can not take place without collisions. In a Landau Fermi liquid, we will will see that the interactions play a non-trivial role that gives rise to "collisionless" collective oscillations of the Fermi surface called "zero sound" (literally zero-collision sound), that are absent in the free Fermi gas[**?**].

To examine the feedback effects of interactions, let us suppose an external potential or field is applied to induce a polarization of the Fermi surface, as illustrated in Fig. 7.3. There are various kinds of external field we can consider - a simple change in the chemical potential

$$\delta\epsilon^0_{\mathbf{p}\sigma} = -\delta\mu, \tag{7.41}$$

which will induce an isotropic enlargement of the Fermi surface, the application of a magnetic field,

$$\delta\epsilon^0_{\mathbf{p}\sigma} = -\sigma\mu_F B. \tag{7.42}$$

which induces a spin polarization. We can also consider the application of a vector potential which couples to the quasiparticle current

$$\delta\epsilon^0_{\mathbf{p}\sigma} = -\mathbf{A}\cdot\frac{e\mathbf{p}}{m}, \tag{7.43}$$

in a translationally invariant system. Notice how, in each of these cases, the applied field couples to a conserved quantity (the particle number, the spin and the current), which is unchanged by interactions. This means that the energy associated with the application of the external field is unchanged by interactions for any quasiparticle configuration $\{n_{\mathbf{p}\sigma}\}$, which guarantees that the coupling to the external field is identical to that of non-interacting particles. This is the reason for the appearance of the unrenormalized mass in (7.43). For each of these cases, there will of course be a feedback effect of the interactions that we now calculate.

From (7.24) the change in the quasiparticle energy will now contain two terms - one due to direct coupling to the external field, the other derived from the induced polarization $\delta n_{\mathbf{p}\sigma}$ of the Fermi surface

$$\delta\epsilon_{\mathbf{p}\sigma} = \delta\epsilon^{(0)}_{\mathbf{p}\sigma} + \sum_{\mathbf{p}'\sigma'} f_{\mathbf{p}\sigma\mathbf{p}'\sigma'}\delta n_{\mathbf{p}'\sigma'}. \tag{7.44}$$

In this case, the equilibrium quasiparticle occupancies become

$$n_{\mathbf{p}\sigma} = f(\epsilon^{(0)}_{\mathbf{p}} + \delta\epsilon_{\mathbf{p}\sigma}) = f(\epsilon^{(0)}_{\mathbf{p}}) + f'(\epsilon^{(0)}_{\mathbf{p}})\delta\epsilon_{\mathbf{p}\sigma}. \tag{7.45}$$

As the temperature is lowered to zero, the derivative of the Fermi function evolves into a delta function $-f'(\epsilon) \sim \delta(\epsilon)$, so that the quasiparticle occupancy is given by

$$n_{\mathbf{p}\sigma} = \overbrace{\theta(-\epsilon^{(0)}_{\mathbf{p}})}^{n^{(0)}_{\mathbf{p}\sigma}} + \overbrace{[-\delta(\epsilon^{(0)}_{\mathbf{p}})\delta\epsilon_{\mathbf{p}\sigma}]}^{\delta n_{\mathbf{p}\sigma}}. \tag{7.46}$$

$\delta n_{\mathbf{p}\sigma} = -\delta(\epsilon^{(0)}_{\mathbf{p}})\delta\epsilon_{\mathbf{p}\sigma}$ represents the polarization of the Fermi surface, which will feed back into the interaction (7.44) as follows

$$\delta n_{\mathbf{p}\sigma} = -\delta(\epsilon^{(0)}_{\mathbf{p}})\delta\epsilon_{\mathbf{p}\sigma}$$

$$\delta\epsilon_{\mathbf{p}\sigma} = \delta\epsilon^{(0)}_{\mathbf{p}\sigma} + \sum_{\mathbf{p}'\sigma'} f_{\mathbf{p}\sigma\mathbf{p}'\sigma'}\delta n_{\mathbf{p}'\sigma'}.$$

The resulting shift in the quasiparticle energies must then satisfy the self-consistency relation:

$$\delta\epsilon_{\mathbf{p}\sigma} = \delta\epsilon^{(0)}_{\mathbf{p}\sigma} - \sum_{\mathbf{p}'\sigma'} f_{\mathbf{p}\sigma\mathbf{p}'\sigma'}\delta(\epsilon^{(0)}_{\mathbf{p}'})\delta\epsilon_{\mathbf{p}'\sigma}. \tag{7.47}$$

This feedback process preserves the symmetry of the external perturbation, but its strength in a given symmetry channel depends on the corresponding Landau paramater. Thus, isotropic charge and spin polarizations of the Fermi surface shown in Fig 7.3(a) and Fig 7.3(b) are fed back via the isotropic charge and magnetic Landau parameters F^s_0 and F^a_0. When the quasiparticle fluid is set into motion at velocity $\vec{u}$, this induces a dipolar polarization of the Fermi surface, shown in (Fig 7.3 (c)), which is fed-back via the dipolar Landau parameter F^s_1. This process is responsible for the renormalization of the effective mass.

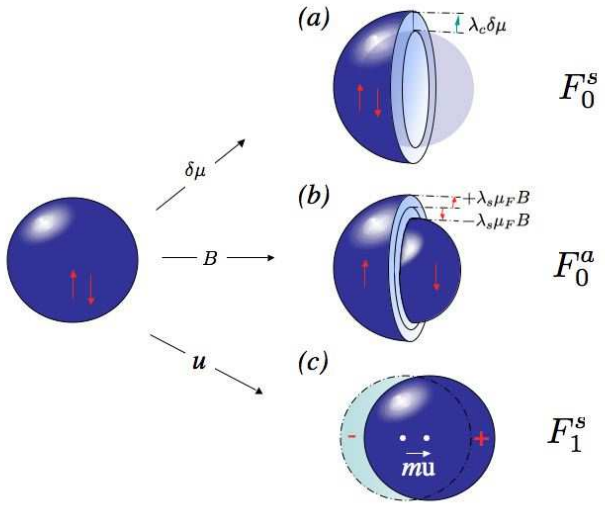


Figure 7.3: Illustrating the polarization of the Fermi surface by (a) a change in chemical potential to produce a isotropic charge polarization (b) application of a magnetic field to produce a spin polarization and (c) the dipolar polarization of the Fermi surface that accompanies a current of quasiparticles. The Landau parameter governing each polarization is indicated on the right hand side.

Consider a change in the quasiparticle potential that has a particular multipole symmetry, so that the "bare" change in quasiparticle energy is

$$\delta\epsilon^{(0)}_{\mathbf{p}\sigma} = v_l Y_{lm}(\hat{\mathbf{p}}) \tag{7.48}$$

where Y_{lm} is a spherical harmonic. The renormalized response of the quasiparticle energy given by

(7.47) must have the same symmetry, but will have a different magnitude t_l:

$$\delta\epsilon_{\mathbf{p}\sigma} = t_l Y_{lm}(\hat{\mathbf{p}}). \tag{7.49}$$

When this is fed back through the interaction, according to (7.47), it produces an additional shift in the quasiparticle energy of given by $\sum_{\mathbf{p}'\sigma'} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\delta n_{\mathbf{p}'\sigma'} = -F_l^s t_l Y_{lm}(\hat{\mathbf{p}})$ (see exercise below), so that the total change in the energy is given by $\delta\epsilon_{\mathbf{p}\sigma} = (v_l - F_l^s t_l)Y_{lm}(\hat{\mathbf{p}})$. Comparing this result with (7.49), we see that

$$t_l = (v_l - F_l^s t_l). \tag{7.50}$$

This is the symmetry resolved version of (7.47). Consequently[3],

$$t_l = \frac{v_l}{1 + F_l^s}. \tag{7.51}$$

We may interpret t_l as the scattering t-matrix associated with the potential v_l. If $F_l^s > 0$ is repulsive, negative feedback occurs which causes the response to be suppressed. This is normally the case in the isotropic channel, where repulsive interactions tend to suppress the polarizability of the Fermi surface. By contrast, if $F_l^s < 0$, corresponding to an attractive interaction, positive feedback enhances the response. Indeed, if F_l^s drops down to the critical value $F_l^s = -1$, an instability will occur and the Landau Fermi surface becomes unstable to a deformation - a process called a "Pomeranchuk" instbality.

A similar calculation can be carried out for a spin-polarization of the Fermi surface, where the shift in the quasiparticle energies are

$$\delta\epsilon^{(0)}_{\mathbf{p}\sigma} = \sigma v_l^a Y_{lm}(\hat{\mathbf{p}}), \qquad \delta\epsilon_{\mathbf{p}\sigma} = \sigma t_l^a Y_{lm}(\hat{\mathbf{p}})$$

Now, the spin-dependent polarization of the Fermi surface feeds back via the spin-dependent Landau parameters so that

$$t_l^a = \frac{v_l^a}{1 + F_l^a}. \tag{7.52}$$

The isotropic response ($l = 0$) corresponds to a simple spin polarization of the Fermi surface. If spin interactions grow to the point where $F_0^a = -1$, the Fermi surface becomes unstable to the formation of a spontaneous spin polarization: this is called a "Stoner" instability, and results in ferromagnetism.

Example 7.3: Calculate the response of the quasiparticle energy to a charge, or spin polarization with a specific multipole symmetry.

[3]Note: in Landau's original formulation[**?**], the Landau parameters were defined without the normalizing factor $(2l + 1)$ in (7.58). With such a normalization the F_l are a factor of $2l + 1$ larger and one must replace $F_l^s \to \frac{1}{2l+1}F_l^s$ in (7.51)

1. Consider a spin-independent polarization of the Fermi surface of the form
$$\delta n_{\mathbf{p}\sigma} = -t_l Y_{lm}(\hat{\mathbf{p}}) \times \delta(\epsilon^{(0)}_{\mathbf{p}})$$
where $Y_{lm}(\hat{\mathbf{p}})$ is a spherical harmonic. Show that the resulting shift in quasiparticle energies is given by
$$\delta\epsilon_{\mathbf{p}\sigma} = -t_l F_l^s\, Y_{lm}(\hat{\mathbf{p}}).$$
2. Determine the corresponding result for a magnetic polarization of the Fermi surface of the form
$$\delta n_{\mathbf{p}\sigma} = -\sigma t_l^a Y_{lm}(\hat{\mathbf{p}}) \times \delta(\epsilon^{(0)}_{\mathbf{p}})$$

Solution:

According to (7.24), the change in quasiparticle energy due to the polarization of the Fermi surface is given by

$$\delta\epsilon_{\mathbf{p}\sigma} = \sum_{\mathbf{p}'\sigma'} f_{\mathbf{p}\sigma,\mathbf{p}',\sigma'}\delta n_{\mathbf{p}'\sigma'}. \tag{7.53}$$

Substituting $\delta n_{\mathbf{p}\sigma} = -t_l Y_{lm}(\hat{\mathbf{p}}) \times \delta(\epsilon^{(0)}_{\mathbf{p}})$, then

$$\delta\epsilon_{\mathbf{p}\sigma} = -t_l \sum_{\mathbf{p}'\sigma'} f_{\mathbf{p}\sigma,\mathbf{p}',\sigma'} Y_{lm}(\hat{\mathbf{p}}') \times \delta(\epsilon^{(0)}_{\mathbf{p}'}). \tag{7.54}$$

Decomposing the interaction into its magnetic and non-magnetic components $f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'} = f^s(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}') + \sigma\sigma' f^a(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}')$, only the non-magnetic survives the spin summation, so that

$$\delta\epsilon_{\mathbf{p}\sigma} = -t_l \times 2\sum_{\mathbf{p}'} f^s(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}')Y_{lm}(\hat{\mathbf{p}}') \times \delta(\epsilon^{(0)}_{\mathbf{p}'}). \tag{7.55}$$

Replacing the summation over momentum by an angular average over the Fermi surface

$$2\sum_{\mathbf{p}'} \delta(\epsilon^{(0)}_{\mathbf{p}'}) \to N^*(0)\int \frac{d\Omega_{\hat{\mathbf{p}}'}}{4\pi}, \tag{7.56}$$

we obtain

$$\begin{aligned}\delta\epsilon_{\mathbf{p}\sigma} &= -t_l \times N^*(0)\int \frac{d\Omega_{\hat{\mathbf{p}}'}}{4\pi} f^s(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}')Y_{lm}(\hat{\mathbf{p}}') \\ &= -t_l \int \frac{d\Omega_{\hat{\mathbf{p}}'}}{4\pi} F^s(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}')Y_{lm}(\hat{\mathbf{p}}')\end{aligned} \tag{7.57}$$

Now we can expand the interaction in terms of Legendre polynomials, which can, in turn be decomposed into spherical harmonics

$$F^s(\cos\theta) = \sum_l (2l+1)F_l^s P_l(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}') = 4\pi\sum_{l,m} F_l^s Y_{lm}(\hat{\mathbf{p}})Y^*_{lm}(\hat{\mathbf{p}}') \tag{7.58}$$

When we substitute this into (7.56) we may use the orthogonality of the spherical harmonics to obtain

$$\delta\epsilon_{\mathbf{p}\sigma} = -t_l \sum_{l'm'} F_{l'}^s Y_{l'm'}(\mathbf{p}) \overbrace{\int d\Omega_{\mathbf{p}'} Y^*_{l'm'}(\hat{\mathbf{p}}')Y_{lm}(\mathbf{p}')}^{\delta_{l'l}\delta_{m'm}}$$

$$= -t_l F_l^s \, Y_{lm}(\hat{\mathbf{p}}). \tag{7.59}$$

For a spin-dependent polarization, $\delta n_{\mathbf{p}\sigma} = -t_l^a \sigma Y_{lm}(\hat{\mathbf{p}})\delta(\epsilon_{\mathbf{p}}^{(0)})$ it is the magnetic part of the interaction that contributes. We can generalize the above result to obtain

$$\delta\epsilon_{\mathbf{p}\sigma} = \sigma t_l^a \times F_l^a \, Y_{lm}(\hat{\mathbf{p}}).$$

7.4.1 Renormalization of Paramagnetism and Compressibility by interactions

The simplest polarization response functions of a Landau Fermi liquid are its "charge" and spin susceptibility.

$$\chi_c = \frac{1}{V}\frac{\partial N}{\partial \mu}, \qquad \chi_s = \frac{1}{V}\frac{\partial M}{\partial B},$$

where V is the volume. Here, we use the term "charge" density to refer to the density response function of the neutral Fermi liquid. These responses involve an isotropic polarization of the Fermi surface. In a neutral fluid, the bulk modulus $\kappa = -V\frac{dP}{dV}$ is directly related to the charge susceptibility per unit volume, $\kappa = \frac{n^2}{\chi_c}$, where $n = N/V$ is the particle density. Thus a smaller "charge" susceptibility implies a stiffer fluid. [4]

When we change the apply a chemical potential or a magnetic field, the "bare" quasiparticle energies respond isotropically.

$$\delta\epsilon_{\mathbf{p}\sigma}^{(0)} = \delta E_{\mathbf{p}\sigma}^{(0)} - \delta\mu = -\sigma\mu_{\rm F}B - \delta\mu. \tag{7.60}$$

Feedback via the interactions renormalizes the response of the full quasiparticle energy

$$\delta\epsilon_{\mathbf{p}\sigma} = -\sigma\lambda_s\mu_{\rm F}B - \lambda_c\delta\mu. \tag{7.61}$$

Since these are isotropic responses, the feedback is transmitted through the $l = 0$ Landau parameters

$$\begin{aligned}\lambda_s &= \frac{1}{1+F_0^a}\\ \lambda_c &= \frac{1}{1+F_0^s}.\end{aligned} \tag{7.62}$$

When we apply a pure chemical potential shift, the resulting change in quasiparticle number is $\delta N = \lambda_c N^*(0)\delta\mu$, so the "charge" susceptibility is given by

$$\chi_c = \lambda_c N^*(0) = \frac{N^*(0)}{1+F_0^s}. \tag{7.63}$$

[4] In a fluid, where $-\partial F/\partial V = P$, the extensive nature of the Free energy guarantees that $F = -PV$, so that the Gibbs free energy $G = F + PV = 0$ vanishes. But $dG = -SdT - Nd\mu + VdP = 0$, so in the ground-state $Nd\mu = VdP$ and hence $\kappa = -V\frac{dP}{dV}\big|_N = -N\frac{d\mu}{dV}\big|_N$, but $\mu = \mu(N/V)$ is a function of particle density alone, so that $-N\frac{d\mu}{dV}\big|_N = \frac{N^2}{V}\frac{d\mu}{dN}\big|_V = \frac{n^2}{\chi_c}$ where $n = N/V$. It follows that $\kappa = \frac{n^2}{\chi_c}$.

Typically, repulsive interactions cause $F_0^s > 0$, reducing the charge susceptibility, making the fluid "stiffer". In ^3He, $F_0^s = 10.8$ at low pressures, which is roughly ten times stiffer than expected, based on its density of states.

A reverse phenomenon occurs to the spin response of Landau Fermi liquids. In a magnetic field, the change in the number of up and down quasiparticles is $\delta n_\uparrow = -\delta n_\downarrow = \frac{1}{2}N^*(0)\mu_F B$. The resulting change in magnetization is $\delta M = \mu_F(\delta n_\uparrow - \delta n_\downarrow) = \lambda_s\mu_F^2 N^*(0)B$, so the spin susceptibility is

$$\chi_s = \lambda_s\mu_F^2 N^*(0) = \frac{\mu_{\rm F}^2 N^*(0)}{1+F_0^a}. \tag{7.64}$$

There are a number of interesting points to be made here:

- The "Wilson" ratio, defined as the ratio between χ_s/γ in the interacting and non-interacting system, is given by
$$W = \frac{\left(\frac{\chi}{\gamma}\right)}{\left(\frac{\chi}{\gamma}\right)_0} = \frac{1}{1+F_0^a}.$$
In the context of ferromagnetism, this quantity is often referred to as the "Stoner enhancement factor" In Landau Fermi liquids with strong ferromagnetic exchange interactions between fermions, F_0^a is negative, enhancing the Pauli susceptibility. This is the origin of the enhancement of the Pauli susceptibility in liquid $He-3$, where $W \sim 4$. In palladium metal Pd, $W = 10$ is even more substantially enhanced[**?**].

- When a Landau Fermi liquid is tuned to the point where $F_0^a \to -1$, $\chi \to \infty$ leading to a ferromagnetic instability. This instability is called a "Stoner instability": it is an example of a ferromagnetic quantum critical point - a point where quantum zero-point fluctuations of the magnetization develop an infinite range correlations in space and time. At such a point, the Wilson ratio will diverge.

7.4.2 Mass renormalization

Using this formulation of the interacting Fermi gas, Landau was able to link the renormalization of quasiparticle mass to the dipole component of the interactions F_1^s. As the fermion moves through the medium, the backflow of the surrounding fluid enhances its effective mass according to the relation

$$m^* = m\left(1+F_1^s\right). \tag{7.65}$$

Another way to understand quasiparticle mass renormalization, is to consider the current carried by a quasiparticle. Whether we are dealing with neutral, or physically charged quasiparticles, the total number of particles is conserved and we can ascribe a particle current current $\mathbf{v}_F = \mathbf{p}_F/m^*$ to each quasiparticle. We can rewrite this current in the form

$$\mathbf{v}_F = \frac{\mathbf{p}_F}{m^*} = \underbrace{\frac{\mathbf{p}_F}{m}}_{\text{bare current}} \overbrace{-\frac{\mathbf{p}_F}{m}\left(\frac{F_1^s}{1+F_1^s}\right)}^{\text{backflow}}. \tag{7.66}$$

The first term is the bare current associated with the original particle, whereas the second term is backflow of the surrounding Fermi sea (Fig. 7.4).

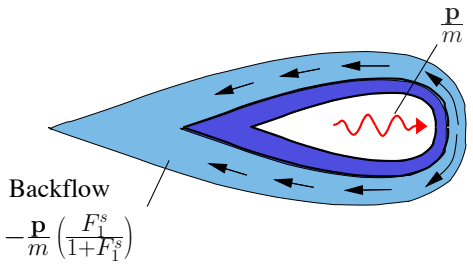


Figure 7.4: Backflow in the Landau Fermi liquid. The particle current in the absence of backflow is $\frac{\mathbf{p}}{m}$. Backflow of the Fermi liquid introduces a reverse current $-\left(\frac{F_1^s}{1+F_1^s}\right)\frac{\mathbf{p}}{m}$.

"Mass renormalization" increases the density of states from $N(0) = \frac{mp_F}{\pi^2} \to N^*(0) = \frac{m^*p_F}{\pi^2}$, i.e it has the effect of compressing the the spacing between the fermion energy levels, which increases the number of quasi-particles that are excited at a given temperature by a factor m^*/m: this enhances the linear specific heat.

$$C_V^* = \frac{m^*}{m}C_V \tag{7.67}$$

where C_V is the Sommerfeld value for the specific heat capacity. Experimentally, the specific heat of Helium-3 *is* enhanced by a factor of 2.8, from which we know that $m^* \approx 3m$.

Landau's original derivation depends on the use of Gallilean invariance. Here we use an equivalent derivation, based on the observation that backflow is a feedback response to the dipolar distortion of the Fermi surface which develops in the presence of a current. This enables us to calculate the mass renormalization in an analogous fashion to the renormalization of the spin susceptibility and compressibility, carried out in (7.4) and (7.4.1), except that now we must introduce the conjugate field to current - that is, a vector potential.

To this end, we imagine that each quasiparticle carries a conserved charge $q = 1$, and that the flow of quasiparticles is coupled to a "fictitious" vector potential $q\mathbf{A} \equiv \mathbf{A}_N$. The microscopic Hamiltonian in the presence of the vector potential is then given by

$$H[\mathbf{A}_N] = \sum_\sigma \int d^3x \frac{1}{2m}\psi_\sigma^\dagger(x)\left[(-i\hbar\nabla - \mathbf{A}_N)^2\right]\psi_\sigma(x) + \hat{V} \tag{7.68}$$

where $\hat{V}$ contains the translationally invariant interactions. Notice that effect of $\mathbf{A}_N$ is to change the momentum of each particle by $-\mathbf{A}_N$, so that $H[\mathbf{A}_N]$ is in fact, the Hamiltonian transformed into

Gallilean reference frame moving at speed $\mathbf{u} = \mathbf{A}_N/m$. Landau's original derivation did infact use the Gallilean equivalence of the Fermi liquid to compute the mass renormalization.

Since the vector potential $\mathbf{A}_N$ is coupled to a conserved quantity - the momentum, we can treat it in the same way as a chemical potential or magnetic field. The linear term in $\mathbf{A}_N$ in the total energy is $\delta\hat{H} = -\mathbf{A}_N \cdot \frac{\hat{\mathbf{P}}}{m}$ where $\hat{\mathbf{P}}$ is the conserved total momentum operator. For a non-interaction system the change in the total energy for a small vector potential at fixed particle occupancies $n_{\mathbf{p}\sigma}$ is

$$\delta E = \langle \delta H\rangle = -\frac{\langle \mathbf{P}\rangle}{m}\cdot\mathbf{A}_N = -\sum_{\mathbf{p}\sigma}(\frac{\mathbf{p}}{m}\cdot\mathbf{A}_N)n_{\mathbf{p}\sigma}. \tag{7.69}$$

Provided the momentum is conserved, this is also the change in the energy of the *interacting* Fermi liquid, at fixed quasiparticle occupancy, i.e. without backflow. In this way, we see that turning on the vector potential changes

$$\epsilon^{(0)}_{\mathbf{p}\sigma} \to \epsilon^{(0)}_{\mathbf{p}\sigma} + \delta\epsilon^{(0)}_{\mathbf{p}\sigma} \tag{7.70}$$

where

$$\delta\epsilon^{(0)}_{\mathbf{p}\sigma} = -\frac{\mathbf{p}}{m}\cdot\mathbf{A}_N = -A_N\frac{p_F}{m}\cos\theta. \tag{7.71}$$

Here, θ is the angle between the vector potential and the quasiparticle momentum. Thus the vector potential introduces a *dipolar potential* around the Fermi surface. Notice how the conservation of momentum guarantees it is the *bare mass* m^* that enters into $\delta\epsilon^{(0)}_{\mathbf{p}\sigma}$.

Now when we take account of the feedback effect caused by the redistribution of quasiparticles in response to this potential, the quasiparticle energy becomes $E_{\mathbf{p}-q\mathbf{A}} = \frac{(\mathbf{p}-\mathbf{A}_N)^2}{2m^*}$. Here, the replacement of $\mathbf{p} \to \mathbf{p} - q\mathbf{A}_N = \mathbf{p} - \mathbf{A}_N$ is guaranteed because the quasiparticle carries the same conserved charge $q = 1$ as the original particles. In this way, we see that in the *presence* of backflow, the change in quasiparticle energy

$$\delta\epsilon_{\mathbf{p}\sigma} = -\frac{\mathbf{p}}{m^*}\cdot\mathbf{A}_N = -A_N\frac{p_F}{m^*}\cos\theta. \tag{7.72}$$

involves the renormalized mass m^*.

Since the vector potential induces a dipolar perturbation to the Fermi surface, using the results from section (7.4), we conclude that backflow feedback effects involve the spin symmetric $l = 1$ Landau Parameter, F_1^s (7.51),

$$\delta\epsilon_{\mathbf{p}\sigma} = \left(\frac{1}{1+F_1^s}\right)\delta\epsilon^{(0)}_{\mathbf{p}\sigma} \tag{7.73}$$

Inserting (7.71) and (7.72) into this relation, we obtain

$$\frac{m}{m^*} = \frac{1}{1+F_1^s} \tag{7.74}$$

or $m^* = m(1+F_1^s)$.

Note that:

- The Landau mass renormalization formula relies on the conservation of particle current when the interactions are adiabatically turned on. In a crystal lattice, although crystal momentum is still conserved, particle current is not conserved and at present, there is no known way of writing down an expression for $\delta\epsilon^{(0)}_{\mathbf{p}\sigma}$ and $\delta\epsilon_{\mathbf{p}\sigma}$ in terms of crystal momentum, that would permit derivation of a mass renormalization formula for electrons in a crystal.

- Since $F^s_1 = N^*(0)f^s_1$ involves the renormalized density of states $N^*(0) = \frac{m^* p_F}{\pi^2}$, the renormalized mass m^* actually appears on both sides of (7.65). If we use (7.31) to rewrite $F^s_1 = \frac{m^*}{m}N(0)f^s_1$, where $N(0) = \frac{mp_F}{\pi^2}$ is the unrenormalized density of states, then we can solve for m^* in terms of m to obtain:

$$m^* = \frac{m}{1 - N(0)f^s_1}. \tag{7.75}$$

  This expression predicts that $m^* \to \infty$ at $N(0)f^s_1 = 1$, i.e that the quasiparticle density of states and hence the specific heat coefficient will diverge if the interactions become too strong. This possibility was first anticipated by Neville Mott, who predicted that in presence of large interactions, fermions will localize, a phenomonon now called a "Mott transition".

There are numerous examples of "heavy electron" systems which lie close to such a localization transition, in which $m^*_e/m_e >> 1$. Quasiparticle masses in excess of $1000m_e$ have been observed via specific heat measurements. In practice, the transition where the mass diverges is usually associated with the development of some other sort of order, such as antiferromagnetism, or solidification. Since the phase transition occurs at zero temperature, in the absence of thermal fluctuations, it is an example of a "quantum phase transition". Such mass divergences have been observed in a variety of different contexts in charged electron systems, but they have also been observed as a second-order quantum phase transition, in the solidification of two-dimensional liquid Helium-3 Mott transition.

7.4.3 Quasiparticle scattering amplitudes

In 8.3 we introduced the quasiparticle interactions $f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}$ as the variation of the quasiparticle energy $\epsilon_{\mathbf{p}\sigma}$ with respect to changes in the quasiparticle occupancy $\delta n_{\mathbf{p}'\sigma'}$, under the condition that the rest of the Fermi sea stays in its ground-state

$$f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'} = \left.\frac{\delta\epsilon_{\mathbf{p}\sigma}}{\delta n_{\mathbf{p}'\sigma'}}\right|_{n_{\mathbf{p}''\sigma''}} = \frac{1}{N^*(0)}\Big[F^s(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}') + \sigma\sigma' F^a(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}')\Big] \tag{7.76}$$

The quantity $f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}$ can be regarded as a bare forward scattering amplitude between the quasiparticles. It proves very useful to define the corresponding quantities when Fermi sea is allowed to respond to the original change in quasiparticle occupancies, as follows:

$$a_{\mathbf{p}\sigma,\mathbf{p}'\sigma'} = \frac{\delta\epsilon_{\mathbf{p}\sigma}}{\delta n_{\mathbf{p}'\sigma'}} = \frac{1}{N^*(0)}\Big[A^s(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}') + \sigma\sigma' A^a(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}')\Big] \tag{7.77}$$

Microscopically, the quantities $a_{\mathbf{p}\sigma\mathbf{p}'\sigma'}$ correspond to the t-matrix for forward-scattering of the quasiparticles. These amplitudes can decoupled in precisely the same way as the Landau interaction

(7.58),

$$\begin{aligned} A^\alpha(\cos\theta) &= \sum_l (2l+1)A^\alpha_l P_l(\cos\theta) \\ &= 4\pi\sum_{l,m} A^\alpha_l Y_{lm}(\hat{\mathbf{p}})Y^*_{lm}(\hat{\mathbf{p}}'), \qquad (\alpha = (s,a)) \end{aligned} \tag{7.78}$$

These two sets of parameters are also governed by the feedback effects of interactions:

$$\boxed{A^\alpha_l = \frac{F^\alpha_l}{1+F^\alpha_l} \qquad (\alpha = s,a)} \tag{7.79}$$

The derivation of this relation follows closely the derivation of relations (7.51) and (7.52); we now repeat the derivation by solving the "Bethe Salpeter" integral equation that links the scattering amplitudes. The change in the quasiparticle energy is

$$\delta\epsilon_{\mathbf{p}\sigma} = f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\delta n_{\mathbf{p}'\sigma'} + \sum_{\mathbf{p}''\sigma''\neq(\mathbf{p}',\sigma')} f_{\mathbf{p}\sigma,\mathbf{p}''\sigma''}\delta n_{\mathbf{p}''\sigma''}, \tag{7.80}$$

where the second term is the induced polarization of the Fermi surface (7.46), $\delta n_{\mathbf{p}''\sigma'} = -\delta(\epsilon^{(0)}_{\mathbf{p}''})\delta\epsilon_{\mathbf{p}''\sigma'}$, so that

$$\delta\epsilon_{\mathbf{p}\sigma} = f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\delta n_{\mathbf{p}'\sigma'} - \sum_{\mathbf{p}''\sigma''} f_{\mathbf{p}\sigma,\mathbf{p}''\sigma''}\delta(\epsilon^{(0)}_{\mathbf{p}''})\delta\epsilon_{\mathbf{p}''\sigma'}. \tag{7.81}$$

Substituting $\delta\epsilon_{\mathbf{p}\sigma} = a_{\mathbf{p}\sigma\mathbf{p}'\sigma'}\delta n_{\mathbf{p}'\sigma'}$ then dividing through by $\delta n_{\mathbf{p}'\sigma'}$, we obtain

$$a_{\mathbf{p}\sigma\mathbf{p}\sigma'} = f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'} - \sum_{\mathbf{p}''\sigma''} f_{\mathbf{p}\sigma,\mathbf{p}''\sigma''}\delta(\epsilon^{(0)}_{\mathbf{p}''})a_{\mathbf{p}''\sigma'\mathbf{p}'\sigma'}. \tag{7.82}$$

This integral equation for the scattering amplitudes is a form of Bethe-Saltpeter equation relating the bare scattering amplitude f to the t-matrix described by a.

Now near the Fermi surface, we can decompose the scattering amplitudes using (7.76) and (7.77), while replacing the momentum summation by an angular integral $\sum_{\mathbf{p}''} \to \frac{1}{2}N^*(0)\int d\epsilon''\int\frac{d\Omega_{\hat{\mathbf{p}}''}}{4\pi}$ so that this equation becomes

$$A^\alpha(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}') = F^\alpha(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}') - \int\frac{d\Omega_{\hat{\mathbf{p}}''}}{4\pi}F^\alpha(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}'')A^\alpha(\hat{\mathbf{p}}''\cdot\hat{\mathbf{p}}') \tag{7.83}$$

If we decompose F and T in terms of spherical harmonics using (7.58) and (7.78) in the second term, we obtain

$$\int\frac{d\Omega_{\hat{\mathbf{p}}''}}{4\pi}F^\alpha(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}'')A^\alpha(\hat{\mathbf{p}}''\cdot\hat{\mathbf{p}}') =$$

$$= (4\pi)^2\sum_{lm,l'm'} F^\alpha_l A^\alpha_{l'}Y_{lm}(\hat{\mathbf{p}})\overbrace{\int\frac{d\Omega_{\hat{\mathbf{p}}''}}{4\pi}Y^*_{lm}(\hat{\mathbf{p}}'')Y_{l'm'}(\hat{\mathbf{p}}'')}^{\delta_{ll'}\delta_{mm'}/(4\pi)}Y^*_{l'm'}(\hat{\mathbf{p}}')$$

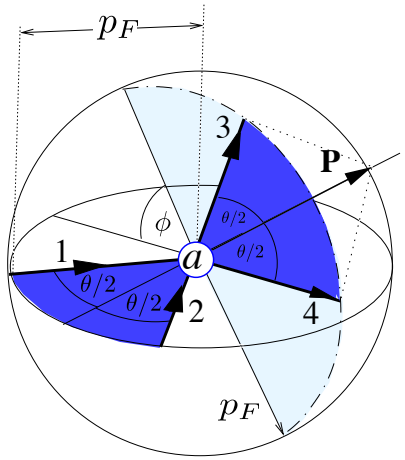


Figure 7.5: Showing the geometry associated with quasiparticle scattering $\mathbf{1}+\mathbf{2}\rightarrow\mathbf{3}+\mathbf{4}$. The momentum transfered in this process is $q=|\mathbf{p}_4-\mathbf{p}_1|=2p_F\sin\theta/2\cos\phi/2$. $\mathbf{P}=\mathbf{p_1}+\mathbf{p_2}$ is the total incoming momentum. Landau parameters determine "forward scattering" processes in which $\phi=0$.

$$= (4\pi)\sum_{lm} F_l^\alpha A_l^\alpha Y_{lm}(\hat{\mathbf{p}})Y_{lm}^*(\hat{\mathbf{p}}') = \sum_l (2l+1)F_l^\alpha A_l^\alpha P_l(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}') \qquad (7.84)$$

Extracting coefficients of the Legendre Polynomials in (7.83), then gives $A_l^\alpha = F_l^\alpha - F_l^\alpha A_l^\alpha$ from which the result

$$A_l^\alpha = \frac{F_l^\alpha}{1+F_l^\alpha} \qquad (\alpha = s,a) \qquad (7.85)$$

follows. The quasiparticle processes described by these scattering amplitudes involve no momentum transfer between the quasiparticles. Geometrically, scattering processes in which $\mathbf{q}=0$ correspond to a situation where the momenta of incoming and outgoing quasiparticles lie in the same plane. Scattering processes which involve situations where the plane defined by the outgoing momenta is tipped through an angle ϕ with respect to the incoming momenta, as shown in Fig. 7.5 involve a finite momentum transfer $q=2p_F|\sin\theta/2\sin\phi/2|$. Provided this momentum transfer is very small compared with the Fermi momentum, i.e $\phi << 1$ then one can extend the t-matrix equation as follows

$$A_l^\alpha(\mathbf{q}) = \frac{F_l^\alpha(\mathbf{q})}{1+F_l^\alpha(\mathbf{q})} \qquad (q << p_F). \qquad (7.86)$$

It is important to realize however, that Landau Fermi liquid theory is however, only really reliable for those processes where $\phi\sim 0$ is small.

7.5 Collective modes

The most common collective mode of a fluid or a gas is "sound". Conventional sound results from collisions amongst particles which redistribute momentum within the fluid - as such, sound is a "low-frequency" phenomenon that operates at frequencies much smaller than the typical quasiparticule scattering rate τ^{-1}, i.e $\omega << \tau^{-1}$ or $\omega\tau << 1$. One of the startling predictions of Landau Fermi liquid theory, is the existence of a collionless collective mode that operates at high frequencies $\omega\tau >> 1$, "zero sound". Zero sound is associated with collective oscillations of the Fermi surface and it does not involve collisions. Whereas conventional sound travels at a speed below the Fermi velocity, zero-sound is "supersonic" traveling at speeds in excess of the Fermi velocity. Historically, the observation of zero-sound in liquid He-3 clinched Landau Fermi liquid, firmly establishing it as a foundation of fermionic many-body physics.

Let us now contrast "zero " and "first" sound. Conventional sound is associated with oscillations in the density of a fluid, and hydrodynamics tells us that

$$u_1^2 = \frac{\kappa}{\rho} = \frac{\kappa}{mn}$$

where $\rho = mn$ is the density of the fluid and $\kappa = -V\frac{\partial P}{\partial V}$ is the bulk modulus. From our previous discussion, $\kappa = \frac{n^2}{\chi_c}$ and $\chi_c = N^*(0)/(1+F_0^s)$, so the velocity of first sound in a Fermi liquid is given by

$$u_1^2 = \frac{n}{m\chi_c} = \frac{n}{mN^*(0)}(1+F_0^s)$$

Replacing $n=\frac{p_F^2}{3\pi^2}$, $N^*(0)=\frac{m^*p_F}{\pi^2}$, and $m=m^*/(1+F_1^s)$ we obtain

$$u_1^2 = \frac{v_F^2}{3}(1+F_0^s)(1+F_1^s) \qquad (7.87)$$

In the non-interacting limit, $u_1 = v_F/\sqrt{3}$ is smaller than the Fermi velocity.

To understand of zero-sound we need to consider variations in the quasiparticle distribution function $n_{\mathbf{p}}(\mathbf{x},t)$. Provided that the characteristic frequency ω and wavevector q of these fluctuations are much respectively smaller than the Fermi energy $\omega << \epsilon_F$ and the Fermi wave-vector $q << k_F$ respectively, then fluctuations in the quasiparticle occupancy can be treated semi-classically, and this leads to a Boltzmann equation

$$\frac{Dn_{\mathbf{p}\sigma}}{Dt} = I[\{n_{\mathbf{p}\sigma}\}]$$

where

$$\frac{Dn_{\mathbf{p}\sigma}}{Dt} = \frac{\partial n_{\mathbf{p}\sigma}}{\partial t} + \dot{\mathbf{x}}\cdot\nabla_{\mathbf{x}} n_{\mathbf{p}\sigma} + \dot{\mathbf{p}}\cdot\nabla_{\mathbf{p}} n_{\mathbf{p}\sigma} \qquad (7.88)$$

is the total rate of change of the quasiparticle occupancy $n_{\mathbf{p}\sigma}(\mathbf{x},t)$, taking into account the movement of quasiparticles through phase space. I is the collision rate. In a semi-classical treatment, the rate of change of momentum and position are determined from Hamilton's equations $\dot{\mathbf{p}} = -\nabla_{\mathbf{x}}\epsilon_{\mathbf{p}}$ and $\dot{\mathbf{x}} = \nabla_{\mathbf{p}}\epsilon_{\mathbf{p}}$, so that

$$\frac{Dn_{\mathbf{p}\sigma}}{Dt} = \frac{\partial n_{\mathbf{p}\sigma}}{\partial t} + \nabla_{\mathbf{p}}\epsilon_{\mathbf{p}}\cdot\nabla_{\mathbf{x}}n_{\mathbf{p}\sigma} - \nabla_{\mathbf{x}}\epsilon_{\mathbf{p}\sigma}\cdot\nabla_{\mathbf{p}}n_{\mathbf{p}\sigma} \tag{7.89}$$

We now consider small fluctuations of the Fermi surface defined by

$$n_{\mathbf{p}}(\mathbf{x},t) = f(\epsilon^{(0)}_{\mathbf{p}}) + e^{i\mathbf{q}\cdot\mathbf{x}-i\omega t}\alpha_{\mathbf{p}\sigma} \tag{7.90}$$

where $\alpha_{\mathbf{p}\sigma}$ is the amplitude of the fluctuations. Now the terms contributing to the total rate of change $Dn_{\mathbf{p}\sigma}/Dt$ are of order $O(\omega\delta n)$, whereas the collision term $I[n] \sim O(\tau^{-1}\delta n)$ is of order the collision rate τ^{-1}. In the high frequency limit, $\omega\tau >> 1$ the collision terms can then be neglected, leading to the collisionless Boltzmann equation:

$$\frac{\partial n_{\mathbf{p}\sigma}}{\partial t} + \nabla_{\mathbf{p}}\epsilon_{\mathbf{p}}\cdot\nabla_{\mathbf{x}}n_{\mathbf{p}\sigma} - \nabla_{\mathbf{x}}\epsilon_{\mathbf{p}\sigma}\cdot\nabla_{\mathbf{p}}n_{\mathbf{p}\sigma} = 0. \tag{7.91}$$

For small periodic oscillations in the Fermi surface, the first two terms in (7.91) can be written

$$\frac{\partial n_{\mathbf{p}\sigma}}{\partial t} + \nabla_{\mathbf{p}}\epsilon_{\mathbf{p}}\cdot\nabla_{\mathbf{x}}n_{\mathbf{p}\sigma} = -i(\omega - \mathbf{v}_F\cdot\mathbf{q})\alpha_{\mathbf{p}\sigma}e^{i\mathbf{q}\cdot\mathbf{x}-i\omega t}$$

In the last term of (7.91), the position dependence of the quasiparticle energies derives from interactions

$$\begin{aligned}\nabla_x\epsilon_{\mathbf{p}\sigma} &= \sum_{\sigma'}\int_{\mathbf{p}'} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\nabla_x n_{\mathbf{p}',\sigma'} \\ &= i\mathbf{q}e^{i\mathbf{q}\cdot\mathbf{x}-i\omega t}\sum_{\sigma'}\int_{\mathbf{p}'} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\alpha_{\mathbf{p}',\sigma'}\end{aligned} \tag{7.92}$$

Replacing $\nabla_{\mathbf{p}}n_{\mathbf{p}\sigma} = \frac{\partial f}{\partial\epsilon}\mathbf{v}_F$, the collisionless Boltzmann equation becomes:

$$(\omega - \mathbf{v}_F\cdot\mathbf{q})\alpha_{\mathbf{p}\sigma} + v_F\cdot\mathbf{q}\left(-\frac{df}{d\epsilon}\right)\sum_{\sigma'}\int_{\mathbf{p}'} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\alpha_{\mathbf{p}',\sigma'} = 0 \tag{7.93}$$

For a mode propagating at speed u, $\omega = uq$. If we express $\mathbf{v}_F.\mathbf{q} = v_F q\cos\theta_{\mathbf{p}}$, and write the mode velocity as a factor s times the Fermi velocity, $u = sv_F$, then this becomes

$$(s - \cos\theta_{\mathbf{p}})\alpha_{\mathbf{p}\sigma} + \cos\theta_{\mathbf{p}}\left(-\frac{df}{d\epsilon}\right)\sum_{\sigma'}\int_{\mathbf{p}'} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\alpha_{\mathbf{p}',\sigma'} = 0 \tag{7.94}$$

We see that the fluctuations in occupancy associated with a zero-sound mode, $\alpha_{\mathbf{p}\sigma} = \eta_\sigma(\hat{\mathbf{p}})\left(-\frac{df}{d\epsilon}\right)$ are proportional to the energy derivative of the Fermi function, and thus confined to within an energy

scale T of the Fermi surface. The function $\eta_\sigma(\hat{\mathbf{p}})$ describes the distribution around the Fermi surface, and this function satisfies the self-consistent relation

$$\eta_\sigma(\mathbf{p}) = \frac{\cos\theta_{\mathbf{p}}}{2(s-\cos\theta_{\mathbf{p}})}\sum_{\sigma'}\int\frac{d\Omega_{\mathbf{p}'}}{4\pi}F_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\eta_\sigma(\hat{\mathbf{p}}') \tag{7.95}$$

For spin-independent zero-sound waves, the right-hand side only involves F^s and can be written

$$\eta(\mathbf{p}) = \frac{\cos\theta_{\mathbf{p}}}{(s-\cos\theta_{\mathbf{p}})}\int\frac{d\Omega_{\mathbf{p}'}}{4\pi}F^s_{\mathbf{p},\mathbf{p}'}\eta(\hat{\mathbf{p}}') \tag{7.96}$$

To illustrate the solution of this equation, consider the case where the interaction is entirely isotropic and spin-independent, so that the only non-vanishing Landau parameter is F^s_0. In this case, the angular function is spin-independent and given by

$$\eta(\theta) = A\frac{\cos(\theta)}{s-\cos(\theta)}$$

where A is a constant. Substituting this form into the integral equation, we obtain the following formula for $s = u/v_F$,

$$A = \int_{-1}^{1}\frac{dcos\theta}{2}\frac{cos\theta}{s-cos\theta}AF^s_0 = AF^s_0\left[-1 + \frac{s}{2}\ln\left(\frac{s+1}{s-1}\right)\right]$$

so that

$$\frac{s}{2}\ln\left(\frac{s+1}{s-1}\right) - 1 = \frac{1}{F^s_0}. \tag{7.97}$$

For large s, the function on the l.h.s. behaves vanishes asymptotically as $1/(3s^2)$, and since the r.h.s. vanishes at large interaction, F^s_0, it follows that for large interaction strength the zero-sound velocity is much greater than v_F,

$$u = sv_F = v_F\sqrt{\frac{F^s_0}{3}}, \qquad (F^s_0 >> 1). \tag{7.98}$$

For small interaction strength, $s \to 1$, and the zero-sound velocity approaches the Fermi velocity.

Experimentally, zero sound has been observed through a variety of methods. Low frequency zero sound couples directly to vibrations at the wall of the fluid, and can be detected directly as a propagating density mode. Zero sound can also be probed at higher frequencies using neutron and X-ray scattering. Neutron scattering experiments find that at high frequencies, the zero sound mode enters back into the particle-hole continuum, where, as a damped excitation, it acquires a "roton" minimum similar to collective modes in bosonic 4-He.

7.6 Charged Fermi Liquids: Landau-Silin theory

One of the most useful extensions of the Landau Fermi liquid theory is to charged Fermi liquids, which underpins our understanding of electrons in metals. Charged Fermi liquids present an additional challenge, because of the long-range Coulomb interaction. The extension of Landau Fermi

liquid theory to incorporate the long-range part of the Coulomb interaction was originally made by Silin[**? ?**]. In neutral Fermi liquids, the existence of well-defined Landau interaction parameters depends on a short-range interaction $V(q)$ with a well-defined zero momentum limit $\mathbf{q} \to \mathbf{0}$ (see also example 8.2). Yet the long-range Coulomb interaction $V(q) = \frac{e^2}{\epsilon_0 q^2}$ is singular as $\mathbf{q} \to 0$. Charged quasiparticles act as sources for an electric potential which satisfy Gauss' law

$$\nabla^2 \phi_P = \frac{e}{\epsilon_0} \sum_{\mathbf{p}} \delta n_{\mathbf{p}\sigma}(\mathbf{x}) \qquad \text{Polarization field} \tag{7.99}$$

The field $\mathbf{E}_P = -\nabla\phi_P$ that this produces polarizes the surrounding quasiparticle fluid to form a *"polarization cloud"* around the quasiparticle which screens its charge, so that the net interaction between screened quasiparticles has a finite range. Nevertheless, this poses a subtle technical problem for screening requires a collective quasiparticle response, yet the Fermi liquid interactions are determined by variation of the quasiparticle energy in response to a change in quasiparticle occupancy against an otherwise frozen (and hence unpolarized) Fermi sea:

$$f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}(\mathbf{x},\mathbf{x}') = \left.\frac{\delta\epsilon_{\mathbf{p}\sigma}(\mathbf{x})}{\delta n_{\mathbf{p}'\sigma'}(\mathbf{x}')}\right|_{\delta n_{\mathbf{p}''\sigma''}=0}$$

In a frozen Fermi sea, the quasiparticle interaction must then be unscreened at large distances, forcing it to be singular as $\mathbf{q} \to 0$.

The solution to this problem was proposed by Silin in 1957. Silin proposed splitting the electric potential ϕ produced by charged particles into two parts: a long range classical polarization field ϕ_P considered above, and a short-range, fluctuating quantum component

$$\phi(\mathbf{x}) = \phi_P(\mathbf{x}) + \delta\phi_Q(\mathbf{x}) \tag{7.100}$$

The quantum component is driven by the virtual creation of electron hole pairs around a charged particle. These processes involve momentum transfer of order the Fermi momentum p_F, are hence localized to within a short distance of order the quasiparticle de Broglie wavelength $\lambda \sim h/p_F$ around the quasiparticle. Silin proposed that these virtual fluctuations in the electric potential introduce a second, short-range component to the quasiparticle interactions. Silin's theory isolates the polarization field as a separate term, so that the quasiparticle energy is written

$$\epsilon_{\mathbf{p}\sigma}(\mathbf{x}) = \epsilon^{(0)}_{\mathbf{p}} + e\phi_P(\mathbf{x}) + \sum_{\mathbf{p}'\sigma'} \tilde{f}_{\mathbf{p}\sigma,\mathbf{p}'\sigma'} \delta n_{\mathbf{p}'\sigma'}(\mathbf{x}) \tag{7.101}$$

In momentum space, the change in the quasiparticle energy is given by

$$\delta\epsilon_{\mathbf{p}\sigma}(\mathbf{q}) = e\phi_P(\mathbf{q}) + \sum_{\mathbf{p}'\sigma'} \tilde{f}_{\mathbf{p}\sigma,\mathbf{p}'\sigma'} \delta n_{\mathbf{p}'\sigma'}(\mathbf{q})$$

However, Gauss' law implies that $e\phi(\mathbf{q}) = \frac{e^2}{\epsilon_0 q^2} \sum_{\mathbf{p}'\sigma'} \delta n_{\mathbf{p}'\sigma'}(\mathbf{q})$. Combining these results together, we see that

$$\delta\epsilon_{\mathbf{p}\sigma}(\mathbf{q}) = \sum_{\mathbf{p}'\sigma'} \left(\frac{e^2}{\epsilon_0 q^2} + \tilde{f}_{\mathbf{p}\sigma,\mathbf{p}'\sigma'} \right) \delta n_{\mathbf{p}'\sigma'}(\mathbf{q})$$

In other words, the effective interaction takes the form (see Fig. 7.6)

$$f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}(\mathbf{q}) = \overbrace{\frac{e^2}{\epsilon_0 q^2}}^{\text{Long range interaction from polarization field}} + \underbrace{\tilde{f}_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}}_{\text{Short-range residual interaction}} \tag{7.102}$$

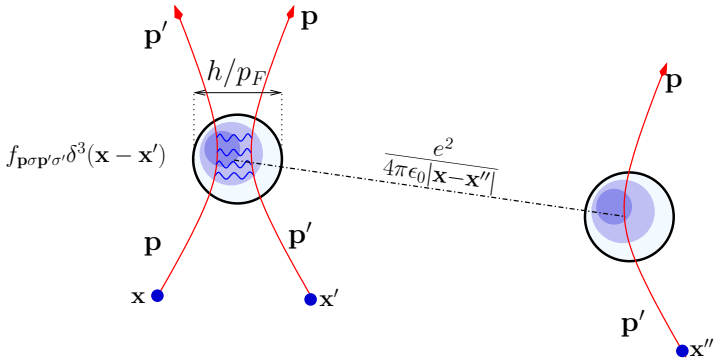


Figure 7.6: Interactions of a charged Fermi liquid. The short-range part of the interaction results from quantum fluctuations of the polarization field (see exercise 8.**??**). The long range component of the interaction derives from the induced polarization field around the quasiparticle.

There are a number of points to emphasize about Silin's theory:

- When the interaction is decomposed in terms of (q-dependent) Landau parameters, the singular interaction only enters into the $l = 0$, spin symmetric component; all the other components are determined by $\tilde{f}_{\mathbf{p}\sigma\mathbf{p}'\sigma'}$, so that

$$F^s_l(\mathbf{q}) = \frac{e^2 N^*(0)}{\epsilon_0 q^2}\delta_{l0} + \tilde{F}^s_l \tag{7.103}$$

  and $F^a_l = \tilde{F}^a_l$.

- The Landau-Silin theory can be derived in a Feynman diagram formalism. In such an approach, the short-range part of the interaction is associated with multiple scattering off the

Coulomb interaction.

- The short-range interaction $\tilde{f}_{\mathbf{p}\mathbf{p}'}$ is a quantum phenomenon, *distinct from classical "Thomas-Fermi" screening of the quasiparticle charge*, which result from the polarizing effects of the long-range, $1/q^2$ component of the interaction.

To illustrate this last point, let us calculate the linear response of the quasiparticle density $\delta\rho(\mathbf{q}) = \chi_c(\mathbf{q})\delta\mu(\mathbf{q})$ to a slowly varying chemical potential $\delta\mu(\mathbf{x}) = \delta\mu(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{x}}$, where $\chi_c(\mathbf{q})$ is the charge susceptibility. In a neutral Fermi liquid, for $q << p_F$, the long-wavelength density response is determined by $\chi_c(\mathbf{q}) \approx \chi_n$, where

$$\chi_n = \frac{N^*(0)}{1+F_0^s}$$

as found in eq. (7.63). In the charged Fermi liquid, we replace $F_0^s \to F_0^s(\mathbf{q}) = \frac{e^2N^*(0)}{\epsilon_0 q^2} + \tilde{F}_0^s$, which gives

$$\chi_c(\mathbf{q}) = \frac{N^*(0)}{1+(\frac{e^2N^*(0)}{\epsilon_0 q^2} + \tilde{F}_0^s)} = \frac{\chi_n}{1+\frac{\kappa^2}{q^2}} = \frac{\chi_n}{1+\frac{e^2}{\epsilon_0 q^2}\chi_n}$$

where $\kappa^2 = \frac{e^2}{\epsilon_0}\chi_n$ defines a "Thomas Fermi" screening length $l_{TF} = \kappa^{-1}$. At large momenta $q >> \kappa$ (distances $x << l_{TF}$), the response is exactly that of the neutral fluid, but at small momenta $q << \kappa$, (distances $x >> l_{TF}$), the charge density response is heavily suppressed.

Historically, the Landau Silin approach changed the way of thinking about metal physics. In early many body theory of the electron gas, the singular nature of the Coulomb interaction was a primary focus, and many body physics in the 1950s was in essence the study of quantum plasmas. With Landau Silin theory, the long-range Coulomb interaction becomes a secondary interest, because this component of the interaction is unrenormalized and can be added in later as an afterthought. This is a major change in philosophy which shifts our interest to the short-range components of the quasiparticle interactions. In essence, the Landau Silin observation liberates us from the singular aspects of the Coulomb interaction, and enables us to treat the physics of strongly correlated electrons as a close companion to other neutral Fermi systems.

Example 7.4: Calculate the scattering t-matrix in Landau-Silin theory to display the screening effect of the long range interaction.

Solution:

If we introduce a small modulation in the quaisparticle occupancy at momentum $\mathbf{p}'$, while "freezing" the rest of the Fermi sea, then the change in the quasiparticle energies will pick up a modulation given by

$$\delta\epsilon_{\mathbf{p}}^{(0)}(\mathbf{q}) = f^s_{\mathbf{p},\mathbf{p}'}(\mathbf{q})\delta n_{\mathbf{p}'}(\mathbf{q}) \tag{7.104}$$

where $f^s_{\mathbf{p},\mathbf{p}'} = \left(\frac{e^2}{\epsilon_0 q^2} + \tilde{f}^s_{\mathbf{p},\mathbf{p}'}\right)$ is the spin symmetric part of the interaction. (For convenience we temporarily drop the spin indices from the subscripts). If we now allow the quasiparticle sea to

polarize in response to the this change in energy, the change in quasiparticle energies will take the form

$$\delta\epsilon_{\mathbf{p}}(\mathbf{q}) = a^s_{\mathbf{p},\mathbf{p}'}(\mathbf{q})\delta n_{\mathbf{p}'}(\mathbf{q}) \tag{7.105}$$

where a^s is the screened quasiparticle interaction to be calculated. At low momenta $\mathbf{q}$ in an isotropic system, both f and a can be expanded in spherical harmonics, as in (7.58), by writing

$$\begin{aligned} f^s_{\mathbf{p},\mathbf{p}'}(\mathbf{q}) &= \frac{4\pi}{N^*(0)}\sum_l F^s_l(\mathbf{q})Y_{lm}(\hat{\mathbf{p}})Y^*_{lm}(\hat{\mathbf{p}}'), \\ a^s_{\mathbf{p},\mathbf{p}'}(\mathbf{q}) &= \frac{4\pi}{N^*(0)}\sum_l A^s_l(\mathbf{q})Y_{lm}(\hat{\mathbf{p}})Y^*_{lm}(\hat{\mathbf{p}}'), \end{aligned} \tag{7.106}$$

For very small $\mathbf{q}$, we can solve for the relationship between T^s_l and F^s_l using the methods of section (7.4.3), which gives

$$A^s_l(\mathbf{q}) = \frac{F^s_l(\mathbf{q})}{1+F_l(\mathbf{q})}$$

But from (7.103), the $\mathbf{q}$ dependence only enters into the $l = 0$ component of the spin-symmetric scattering, where $F_0(\mathbf{q}) = \frac{e^2N^*(0)}{\epsilon_0 q^2} + \tilde{F}_0$ so that

$$A^s_0(\mathbf{q}) = \frac{\frac{e^2N^*(0)}{\epsilon_0 q^2} + \tilde{F}_0}{1+\frac{e^2N^*(0)}{\epsilon_0 q^2} + \tilde{F}_0} = \frac{\kappa^2/(1+\tilde{F}^s_0)}{(\kappa^2+q^2)} + A_0^{s(neutral)}$$

where $A_0^{neutral} = \frac{F^s_0}{1+\tilde{F}^s_0}$ is the $l = 0$ scattering t-matrix of the equivalent neutral Fermi liquid. Since all other components are unchanged by the long-range Coulomb interaction, it follows that the interaction t-matrix of the charged Fermi liquid is a sum of the original neutral interaction, plus a screened Coulomb correction:

$$a_{\mathbf{p}\sigma,\mathbf{p}'\sigma}(\mathbf{q}) = \frac{1}{(1+\tilde{F}^s_0)^2}\frac{e^2}{\epsilon_0(q^2+\kappa^2)} + a^{(neutral)}_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}. \tag{7.107}$$

Note how the residual "Coulomb" part of the t-matrix is heavily suppressed when $\tilde{F}^s_0$ becomes large.

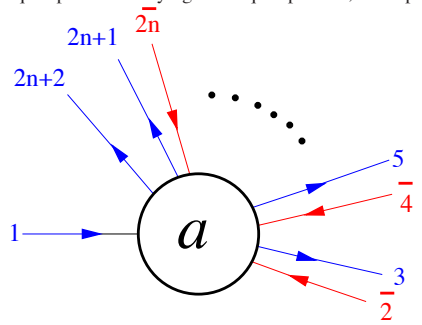
7.7 Inelastic Quasiparticle Scattering

7.7.1 Heuristic derivation.

In this section we show how the Pauli exclusion principle limits the phase for scattering of quasiparticles in a Landau Fermi liquid, giving rise to a scattering rate with a quadratic dependence on excitation energy and temperature

$$\frac{1}{\tau} \propto [\epsilon^2 + \pi^2T^2].$$

The dominant decay mode of a quasiparticle is into three quasiparticles. There are also higher order processes that involve a quasiparticle decaying into a quasiparticle, and n particle-hole pairs:



We'll see that the phase space for these higher order decay processes vanishes with a high power of the energy ($\propto \epsilon^{2n+1}$), allowing us to neglect them relative to the leading process at low temperature and energy. For our discussion, we will denote a hole in the quasiparticle state $\mathbf{j}$ as $\bar{\mathbf{j}}$, denoting the quasihole energy by $\tilde{\epsilon}_j = -\epsilon_j > 0$. By the Golden Rule, the rate of decay into n particle-hole pairs is

$$\Gamma_{2n+1}(\epsilon_1) \sim \frac{2\pi}{\hbar} \sum_{\substack{2,3,\ldots 2n+2 \\ \tilde{\epsilon}_2,\epsilon_3\cdots>0}} |a(1;\bar{2},3,\ldots,2n+2)|^2 \delta[\epsilon_1 - (\tilde{\epsilon}_2 + \epsilon_3 + \tilde{\epsilon}_4 \cdots + \epsilon_{2n+2})] \tag{7.108}$$

where $a(1;\bar{2},3,\ldots 2n+1)$ is the amplitude for the scattering process, $\bar{\epsilon}_2, \bar{\epsilon}_4, \ldots \bar{\epsilon}_{2n} \ldots$ denote the energies of the outgoing quasiholes and $\epsilon_3, \epsilon_5 \ldots \epsilon_{2n+1}, \epsilon_{2n+2}$ denote the energies of the outgoing quasiparticles. The energies of the final state quasi- particles and holes must all be positive, while also summing up to give the initial energy. When the incoming particle is close to the Fermi energy, ϵ and the all final state energies $\epsilon_1 > \epsilon_i > 0$ must also lie close to the Fermi energy, so so we can replace $|a|^2$ by an appropriate Fermi surface average

$$\langle |a_{2n+1}|^2 \rangle = \sum_{2,3,\ldots 2n+2} |a(1;\bar{2},3,\ldots 2n+2)|^2 \delta(\tilde{\epsilon}_2) \ldots \delta(\epsilon_{2n+1}).$$

to obtain [5]

$$\Gamma_{2n+1}(\epsilon) \sim \frac{2\pi}{\hbar} \langle |a_{2n+1}|^2 \rangle \int_0^\infty d\tilde{\epsilon}_2 \ldots d\epsilon_{2n+1} \delta[\epsilon - (\tilde{\epsilon}_2 + \ldots \epsilon_{2n+1})] \propto \frac{\epsilon^{2n}}{(2n)!}. \tag{7.109}$$

[5] Formally this is done by inserting $1 = \prod_{i=1}^{2n+1} \int_{-\infty}^{\infty} d\epsilon_i \delta(\epsilon_i)$ into (7.108),

In this way[6], the phase space for decay into $2n+1$ quasiparticles vanishes as ϵ_1^{2n}. This means that near the Fermi surface, quasiparticle decay is dominated by the decay into two quasi-particles and a quasihole, denoted by $\mathbf{1} \longrightarrow \bar{\mathbf{2}} + \mathbf{3} + \mathbf{4}$ as illustrated in Fig. (7.7).

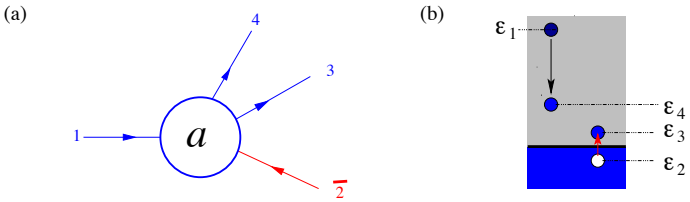


Figure 7.7: Decay of a quasiparticle into two quasiparticles and a quasihole. (a) Scattering process. (b) Energies of final states.

The decay rate for this process is given by

$$\Gamma(\epsilon) = \frac{2\pi}{\hbar} \langle |a_3|^2 \rangle \frac{\epsilon^2}{2}$$

On dimensional grounds, we expect the averaged squared matrix element to scale as $\langle |a_3|^2 \rangle \sim \frac{w^2}{\epsilon_F}$, where w is a dimensionless measure of the strength of the scattering, so that $\Gamma \sim \frac{2\pi}{\hbar} \frac{\epsilon^2}{\epsilon_F}$.

7.7.2 Detailed calculation of three body decay process

We now present a more detailed calculation of quasiparticle decay, deriving a result that was first obtained by Abrikosov and Khalatnikov in 1957[**?**]. The amplitude to produce an outgoing hole in state $\bar{\mathbf{2}}$ is equal to the amplitude to absorb an incoming particle in state $\mathbf{2}$, so we denote

$$a(\mathbf{1} \longrightarrow \bar{\mathbf{2}} + \mathbf{3} + \mathbf{4}) = a(\mathbf{1} + \mathbf{2} \longrightarrow \mathbf{3} + \mathbf{4}) \equiv a(\mathbf{1}, \mathbf{2}; \mathbf{3}, \mathbf{4})$$

Using Fermi's golden rule, the net scattering rate into state $\mathbf{1}$ is given by

$$I[n_{\mathbf{p}}] = \frac{2\pi}{\hbar} \sum_{2,3,4} |a(\mathbf{1},\mathbf{2};\mathbf{3},\mathbf{4})|^2 \Big[\overbrace{(1-n_2)n_3 n_4(1-n_1)}^{\bar{\mathbf{2}}+\mathbf{3}+\mathbf{4} \to \mathbf{1}} - \overbrace{n_1 n_2 (1-n_3)(1-n_4)}^{\mathbf{1} \to \bar{\mathbf{2}}+\mathbf{3}+\mathbf{4}} \Big]$$

[6] This last integral can be done by regarding the ϵ_r as the differences $\epsilon_j = s_j - s_{j-1}$ between an ordered set of co-ordinates $s_{2n+1} > s_{2n} \cdots > s_1$ where $s_0 = 0$, so that

$$\int_0^\infty \underbrace{d\epsilon_1 \ldots d\epsilon_{2n+1}}_{=ds_1 \ldots ds_{2n+1}} \delta[\epsilon - \overbrace{(\epsilon_1 + \epsilon_2 + \ldots \epsilon_{2n+1})}^{s_{2n+1}}] = \int_0^\infty ds_{2n+1} \delta(\epsilon - s_{2n+1}) \int_0^{s_{2n+1}} ds_{2n} \ldots \int_0^{s_2} ds_1 = \frac{\epsilon^{2n}}{(2n)!}.$$

$$\times \quad (2\pi\hbar)^3\delta^{(3)}(\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_3-\mathbf{p}_4)\,\delta(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4) \tag{7.110}$$

where $\sum_2 \equiv \int \frac{d^3p}{(2\pi\hbar)^3}$ denotes a sum over final state momenta, and the delta functions impose the conservation of momentum and energy, respectively. The terms inside the square brackets determine the *à priori* probabilities for the scattering process. For scattering into state **1**, the initial states must be occupied and the final state must be empty, so the à priori probability is $(1-n_2)n_3n_4 \times (1-n_1)$, where $(1-n_2)$ is the probability that the quasihole state $\bar{\mathbf{2}}$ is occupied and n_3n_4 is the probability that **3** and **4** are occupied, while $(1-n_1)$ is the probability that the final quasiparticle state **1** is empty. The second term in the brackets describes the scattering out of state **1**, and can be understood in a similar way.

In thermal equilibrium, the scattering rate vanishes $I[n_{\mathbf{p}}^{(0)}] = 0$ and for small deviations from equilibrium, we may expand the collision integral to linear order in $\delta n_{\mathbf{p}} = n_{\mathbf{p}} - n_{\mathbf{p}}^{(0)}$, identifying the coefficient as the quasiparticle decay rate as follows, $I[n_{\mathbf{p}}] = -\Gamma\delta n_1 + O(\delta n_{\mathbf{p}}^2)$, where $\Gamma = -\frac{\delta I}{\delta n_1}$, or

$$\begin{aligned}\Gamma &= \frac{2\pi}{\hbar}\sum_{2,3,4}|a(1,2;3,4)|^2\Big[n_2(1-n_3)(1-n_4)+(1-n_2)n_3n_4\Big]\\ &\times \quad (2\pi\hbar)^3\delta(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)\delta^{(3)}(\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_3-\mathbf{p}_4).\end{aligned} \tag{7.111}$$

The occupation factors in the square brackets impose the Fermi statistics. These terms are easiest to understand at absolute zero, where $n_{\mathbf{p}} = \theta(-\epsilon_{\mathbf{p}})$ restricts $\epsilon_{\mathbf{p}} < 0$ and $1-n_{\mathbf{p}} = \theta(\epsilon_{\mathbf{p}})$ restricts $\epsilon_{\mathbf{p}} > 0$. The first term $n_2(1-n_3)(1-n_4)$ enforces the constraint that the excitation energies $-\epsilon_2, \epsilon_3,\ \epsilon_4 > 0$ are all positive. (Recall that the ϵ_j refer to quasiparticle energies, so $-\epsilon_2 = \bar{\epsilon}_2$ is the excitation energy of the outgoing hole in state $\bar{\mathbf{2}}$.) At absolute zero, the second term $(1-n_2)n_3n_4$ is zero unless the excitation energies are negative, and vanishes when $\epsilon_1 > 0$. Now the delta function $\delta(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)$ enforces energy conservation, $\bar{\epsilon}_2+\epsilon_3+\epsilon_4 = \epsilon_1$. Together with the requirement that the scattered quasiparticle energies are positive, this term forces all three excitation $|\epsilon_{2,3,4}|$ energies to be smaller than ϵ. In this way, we see that for small ϵ, the final quasiparticle states must lie very close to the Fermi momentum.

With this understanding, at low tempertures, we can replace the integrals over three dimensional momentum by the product of an energy and an angular integral over the direction of the momenta on the Fermi surface:

$$\sum_{\mathbf{p}'} \to \frac{N^*(0)}{2}\int\frac{d\Omega_{\hat{\mathbf{p}}'}}{4\pi}\times\int d\epsilon',$$

This factorization between the energy and momentum degrees of freedom is a hallmark of the Landau Fermi liquid. Using it, we can factorize (7.111) into two parts

$$\Gamma = \frac{2\pi}{\hbar}\overbrace{\big\langle|a_3|^2\big\rangle}^{\text{angular average}}\times\overbrace{\Big\langle n_2(1-n_3)(1-n_4)+(1-n_2)n_3n_4\Big\rangle_{\epsilon_2,\epsilon_3,\epsilon_4}}^{\text{energy phase space integral}}, \tag{7.112}$$

where

$$\big\langle|a_3|^2\big\rangle = \left(\frac{N^*(0)}{2}\right)^3\int\frac{d\Omega_2 d\Omega_3 d\Omega_4}{(4\pi)^3}|a(1,2;3,4)|^2(2\pi\hbar)^3\delta^{(3)}[p_F(\hat{\mathbf{n}}_1+\hat{\mathbf{n}}_2-\hat{\mathbf{n}}_3-\hat{\mathbf{n}}_4)]$$

is the angular average and

$$\langle\ldots\rangle_{\epsilon_2,\epsilon_3,\epsilon_4} = \int d\epsilon_2 d\epsilon_3 d\epsilon_4\delta(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)[\ldots]$$

is the energy phase space integral. At absolute zero, the argument of the phase space integral restricts the final states to have positive excitation energies, giving $\frac{\epsilon_1^2}{2}$, as obtained from (7.109) for $n=1$. At finite temperature (see example), thermal broadening leads to an additional quadratic temperature dependence to the phase space integral[7]

$$\Big\langle\ n_2(1-n_3)(1-n_4)+(1-n_2)n_3n_4\Big\rangle_{\epsilon_{2,3,4}} = \frac{1}{2}\left(\epsilon_1^2+(\pi k_BT)^2\right)$$

To calculate the average squared matrix element, it is convenient to first ignore the spin of the quasiparticle. To evaluate the angular integral, we need to consider the geometry of the scattering process near the Fermi surface, which is illustrated in Fig. (7.5). At low temperatures, all initial and final momenta lie on the Fermi surface, $|\mathbf{p}_j| = p_F$. The total momentum in the particle-particle channel is $\mathbf{P} = \mathbf{p}_1+\mathbf{p}_2$. Suppose the angle between $\mathbf{p}_1$ and $\mathbf{p}_2$ is θ, so that each of these momenta subtends an angle $\theta/2$ with $\mathbf{P}$ as shown in Fig. 7.5, then $|\mathbf{P}| = 2p_F\sin\theta/2$. Now since the total momentum is conserved, $\mathbf{p}_3+\mathbf{p}_4 = \mathbf{P}$ also, so that $|\mathbf{p}_3+\mathbf{p}_4| = 2p_F\sin\theta/2$, which means that $\mathbf{p}_3$ and $\mathbf{p}_4$ also subtend an angle $\theta/2$ with $\mathbf{P}$. However, in general, the planes defined by $\mathbf{p}_{1,2}$ and $\mathbf{p}_{3,4}$ are not the same, and we denote the angle between them by ϕ. In general, the scattering amplitude $a(\theta,\phi)$ will be a function of the two angles, θ and ϕ. In this way, we can parameterize the scattering amplitude by $a(\theta,\phi)$.

A detailed evaluation of the angular integral $\langle|a_3|^2\rangle$ (see example 8.4), leads to the result

$$\langle|a_3|^2\rangle = \frac{1}{2}\times\pi^2\left(\frac{N^*(0)\hbar}{2p_F}\right)^3\left\langle\frac{|a(\theta,\phi)|^2}{2\cos\theta/2}\right\rangle_\Omega \tag{7.113}$$

where

$$\left\langle\frac{|a(\theta,\phi)|^2}{2\cos\theta/2}\right\rangle_\Omega \equiv \int\frac{d\cos\theta d\phi}{4\pi}\left(\frac{|a(\theta,\phi)|^2}{2\cos\theta/2}\right)$$

denotes a weighted, normalized angular average of the scattering rate over the Fermi surface. For identical spinless particles, the final states with scattering angle ϕ and $\phi+\pi$ are are indistinguishable, and the pre-factor of one half is introduced into (7.113) to take into account the overcounting that occurs when we integrate from $\phi = 0$ to $\phi = 2\pi$.

The complete scattering rate for a spinless quasiparticle is then given by

$$\Gamma = \frac{2\pi}{\hbar}\times\left\langle\frac{\frac{1}{2}|a(\theta,\phi)|^2}{2\cos\theta/2}\right\rangle_\Omega\pi^2\left(\frac{N^*(0)\hbar}{2p_F}\right)^3\times\left(\frac{\epsilon^2+(\pi k_BT)^2}{2}\right) \tag{7.114}$$

[7] The first term in the phase space integral corresponds to the decay $1\to\bar{2}+3+4$ of a quasiparticle, while the second term describes the regeneration of quasiparticles via the reverse process $\bar{2}+3+4\to 1$. The classic treatment of the quasiparticle decay given by Abrikosov and Khaltnikov[**? ?**], reproduced in Pines and Noziéres and in Mahan, only includes the first process, which introduces an additional factor $1/(1+e^{-\beta\epsilon_1})$ into this expression.

Let us now consider how this answer changes when we reinstate the spin of the quasiparticles. In this case, we must sum over the two spin orientations of quasiparticle 2, corresponding the case where the spin of 1 and 2 are either parallel ($A_{\uparrow\uparrow}$) or antiparallel ($A_{\uparrow\downarrow}$). When the spins of the two quasiparticles are parallel they are indistinguishable and we must keep the factor of $\frac{1}{2}$, but when the spins are antiparallel, the particles are distinguishable and this factor is omitted. So to take account of spin, we must replace

$$\frac{1}{2}|a(\theta,\phi)|^2 \to \frac{1}{2}|a_{\uparrow\uparrow}(\theta,\phi)|^2 + |a_{\uparrow\downarrow}(\theta,\phi)|^2$$

in (7.114). Following the original convention of Abrikosov and Khalatnikov [**?**], we denote

$$\frac{2\pi}{\hbar}\left(|a_{\uparrow\downarrow}(\theta,\phi)|^2 + \frac{1}{2}|a_{\uparrow\uparrow}(\theta,\phi)|^2\right) = 2W(\theta,\phi).$$

Applying these substutions to (7.114), and writing $N^*(0) = m^* p_F/(\pi^2\hbar^3)$, we obtain

$$\Gamma = \frac{(m^*)^3}{8\pi^4\hbar^6}\left\langle \frac{W(\theta,\phi)}{2\cos\theta/2}\right\rangle_\Omega \times (\epsilon^2 + (\pi k_B T)^2) \tag{7.115}$$

This result was originally obtained by Abrikosov and Khalatnikov in 1957[**?**]. An alternative way to rewrite this expression is identify the normalized scattering amplitudes $N^*(0)a_{\alpha\beta}(\theta,\phi) = A_{\alpha\beta}(\theta,\phi) \equiv A_{\alpha\beta}(\mathbf{q})$ with the dimensionless t-matrix introduced in section (7.4.3). From this we see that the average matrix elements can be written in terms of a dimensionless parameter w^2

$$w^2 = \left\langle \frac{|A_{\uparrow\downarrow}(\theta,\phi)|^2 + \frac{1}{2}|A_{\uparrow\uparrow}(\theta,\phi)|^2}{2\cos\theta/2}\right\rangle_\Omega .$$

In many strongly interacting systems, w is close to unity. Using this notation, the scattering rate (7.115) can be written in the form

$$\Gamma = \frac{2\pi}{\hbar}\overbrace{\left(\frac{w^2}{16\epsilon_F}\right)}^{\langle|a_3|^2\rangle}\left[\frac{\epsilon^2 + (\pi k_B T)^2}{2}\right] \tag{7.116}$$

Apart from the factor of 16 in the denominator, this is what we guessed on dimensional grounds.

There are two important regimes of behaviour to note:

- $|\epsilon_{\mathbf{p}}| << \pi k_B T$: $\Gamma \propto T^2$. Near the Fermi surface, quasiparticles are thermally excited, with a T^2 scattering rate that is independent of energy.
- $|\epsilon_{\mathbf{p}}| >> \pi k_B T$: $\Gamma \propto \epsilon_{\mathbf{p}}^2$. For higher energy quasiparticles, the scattering rate is quadratically dependent on energy.

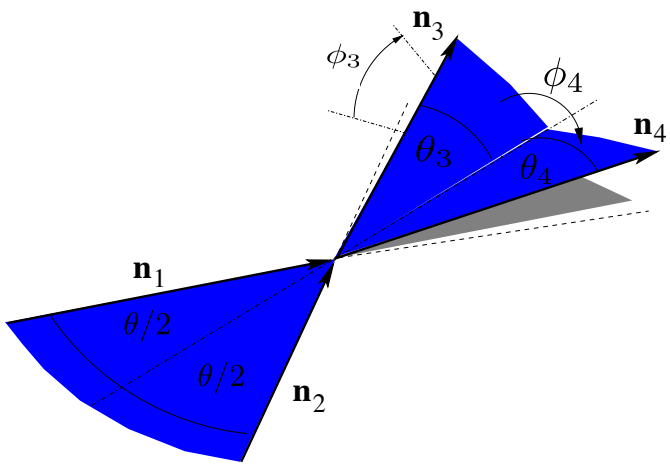


Figure 7.8: Co-ordinate system used to calculate the angular average of the scattering amplitude.

Example 7.5: Calculate the angular average of the scattering amplitude

$$\left\langle|a_3|^2\right\rangle = \left(\frac{N^*(0)}{2}\right)^3 \int \frac{d\Omega_2 d\Omega_3 d\Omega_4}{(4\pi)^3}|a(1,2;3,4)|^2(2\pi\hbar)^3\delta^{(3)}[p_F(\hat{\mathbf{n}}_1+\hat{\mathbf{n}}_2-\hat{\mathbf{n}}_3-\hat{\mathbf{n}}_4)]$$

in the dominant quasiparticle decay processes.

Solution: We first replace $\delta^{(3)}[p_F(\hat{\mathbf{n}}_1+\hat{\mathbf{n}}_2-\hat{\mathbf{n}}_3-\hat{\mathbf{n}}_4)] \to \frac{1}{p_F^3}\delta^{(3)}[\hat{\mathbf{n}}_1+\hat{\mathbf{n}}_2-\hat{\mathbf{n}}_3-\hat{\mathbf{n}}_4]$, so that

$$\left\langle|a_3|^2\right\rangle = \left(\frac{N^*(0)\hbar}{4p_F}\right)^3 \int d\Omega_2 d\Omega_3 d\Omega_4 \delta^{(3)}[\hat{\mathbf{n}}_1+\hat{\mathbf{n}}_2-\hat{\mathbf{n}}_3-\hat{\mathbf{n}}_4]|a(1,2;3,4)|^2 \tag{7.117}$$

To carry out the angular integral, we use polar co-ordinates for $\hat{\mathbf{n}}_2 \equiv (\theta,\phi_2)$, $\hat{\mathbf{n}}_3 \equiv (\theta_3,\phi_3)$ and $\hat{\mathbf{n}}_4 = (\theta_4,\phi_4)$, (as illustrated in Fig. 7.8), where θ and ϕ_2 are the polar angles of $\mathbf{n_2}$ relative to $\mathbf{n}_1$, $\theta_{3,4}$ are the angles between $\hat{\mathbf{n}}_{3,4}$ and the direction of the total momentum $\hat{\mathbf{P}}$, while ϕ_3 is the azimuthal angle of $\mathbf{n_3}$ measured relative to the plane defined by $\hat{\mathbf{n}}_1$ and $\hat{\mathbf{n}}_2$ and ϕ_4 is azimuthal angle of $\mathbf{n_4}$ measured relative to the common plane of $\hat{\mathbf{n}}_3$ and $\hat{\mathbf{P}}$. The delta function in the integral will force $\hat{\mathbf{n}}_3$ and $\hat{\mathbf{n}}_4$ to lie in a place, so that ultimately, we only need to know the dependence of the amplitude $a(\theta,\phi_3)$ on θ and ϕ_3.

Taking the z-axis to lie along $\hat{\mathbf{P}}$ and choosing the y axis to lie along $\hat{\mathbf{P}}\times\hat{\mathbf{n}}_3$, then in this co-ordinate system, $\hat{\mathbf{n}}_1+\hat{\mathbf{n}}_2 = (0,0,2\cos\theta/2)$, $\hat{\mathbf{n}}_3 = (\sin\theta_3,0,\cos\theta_3)$ and $\hat{\mathbf{n}}_4 =$

$(\sin\theta_4\cos\phi_4, \sin\theta_4\sin\phi_4, \cos\theta_4)$, so that

$$\begin{aligned} & \hat{\mathbf{n}}_3 + \hat{\mathbf{n}}_4 - \hat{\mathbf{n}}_1 - \hat{\mathbf{n}}_2 \\ = \; & (\sin\theta_3 + \sin\theta_4\cos\phi_4, \sin\theta_4\sin\phi_4, \cos\theta_3 + \cos\theta_4 - 2\cos(\theta/2)) \end{aligned}$$

Factorizing the three dimensional delta function into its x, y and z components gives

$$\begin{aligned} & \delta^{(3)}[(\hat{\mathbf{n}}_1 + \hat{\mathbf{n}}_2 - \hat{\mathbf{n}}_3 - \hat{\mathbf{n}}_4)] \\ = \; & \delta[\sin\theta_3 + \sin\theta_4\cos\phi_4]\delta[\sin\theta_4\sin\phi_4]\delta[\cos\theta_3 + \cos\theta_4 - 2\cos(\theta/2)] \end{aligned}$$

Integrating over $d\Omega_4 = sin\theta_4 d\theta_4 d\phi_4$ forces $\phi_4 = \pi$ and $\theta_4 = \theta_3$ (note that $\phi_4 = 0$ satisfies the second delta function, but this then requires that $\sin\theta_3 = -\sin\theta_4$ which is not possible when $\theta_{3,4} \in [0, \pi]$). Resolving the delta functions around these points, we may write

$$\delta[\sin\theta_3 + \sin\theta_4\cos\phi_4]\delta[\sin\theta_4\sin\phi_4] = \frac{\delta(\theta_3 - \theta_4)}{\cos\theta_4}\frac{\delta(\phi_4 - \pi)}{\sin\theta_4}.$$

When we carry out the integral over $d\Omega_4 = \sin\theta_4 d\theta_4 d\phi_4$, we then obtain

$$\int d\Omega_4 \delta^{(3)}[\hat{\mathbf{n}}_1 + \hat{\mathbf{n}}_2 - \hat{\mathbf{n}}_3 - \hat{\mathbf{n}}_4]|a(\theta,\phi_3)|^2 = \frac{1}{\cos\theta_3}\delta[2\cos\theta_3 - 2\cos(\theta/2)]|a(\theta,\phi_3)|^2$$

Integrating over $d\Omega_3 = d\phi_3 d\cos\theta_3$ imposes $\theta_3 = \theta/2$, so that

$$\int d\Omega_3 d\Omega_4 \delta^{(3)}[\hat{\mathbf{n}}_1 + \hat{\mathbf{n}}_2 - \hat{\mathbf{n}}_3 - \hat{\mathbf{n}}_4]|a(\theta,\phi_3)|^2 = \int \frac{d\phi_3}{2\cos\theta/2}|a(\theta,\phi_3)|^2$$

The azimuthal angle ϕ_2 of $\hat{\mathbf{n}}_2$ about $\mathbf{n_1}$ does not enter into the integral, so we may integrate over this angle, and write the measure $d\Omega_2 \equiv 2\pi d\cos\theta$. The complete angular integral is then

$$\int d\Omega_2 d\Omega_3 d\Omega_4 \delta^{(3)}[\hat{\mathbf{n}}_1 + \hat{\mathbf{n}}_2 - \hat{\mathbf{n}}_3 - \hat{\mathbf{n}}_4]|a(\theta,\phi_3)|^2 = 2\pi\int \frac{d\phi_3 d\cos\theta}{2\cos\theta/2}|a(\theta,\phi_3)|^2.$$

Substituting this result into (7.117), the complete angular average is then

$$\left\langle |a_3|^2 \right\rangle = \pi^2\left(\frac{N^*(0)\hbar}{2p_F}\right)^3 \int \frac{d\cos\theta d\phi}{4\pi}\frac{|a(\theta,\phi)|^2}{2\cos\theta/2}$$

where we have relabelled ϕ_3 as ϕ. Notice (i) that the weighted angular average is normalized, so that if $|a(\theta,\phi)|^2 = |a|^2$ is constant, $\langle |a_3|^2\rangle = \pi^2\left(\frac{N^*(0)\hbar}{2p_F}\right)^3|a|^2$, and that (ii) since the denominator in the average vanishes for $\theta = \pi$, the angular average contributing to the quasiparticle decay is weighted towards large angle scattering events in which the outgoing quasiparticles have opposite momenta $\mathbf{p}_3 = -\mathbf{p}_4$. This feature is closely connected with the Cooper pair instability discussed in Chapter 14.

Example 7.6: Compute the energy phase space integral

$$I(\epsilon,T) = \int_{-\infty}^{\infty} d\epsilon_2 d\epsilon_3 d\epsilon_4 \delta(\epsilon + \epsilon_2 - \epsilon_3 - \epsilon_4)[n_2(1-n_3)(1-n_4) + (1-n_2)n_3 n_4],$$

where $n_i \equiv f(\epsilon_i) = 1/(e^{\beta\epsilon}+1)$ denotes the Fermi function evaluated at energy ϵ_i

Solution: As a first step, we make a change of variable $\epsilon_2 \to -\epsilon_2$, so that the integral becomes

$$\begin{aligned} I(\epsilon,T) &= \int_{-\infty}^{\infty} d\epsilon_2 d\epsilon_3 d\epsilon_4 \delta(\epsilon - (\epsilon_2 + \epsilon_3 + \epsilon_4))[(1-n_2)(1-n_3)(1-n_4) + n_2 n_3 n_4] \\ &= \int_{-\infty}^{\infty} d\epsilon_2 d\epsilon_3 d\epsilon_4 \delta(\epsilon - (\epsilon_2 + \epsilon_3 + \epsilon_4))[n_2 n_3 n_4 + \{\epsilon \leftrightarrow -\epsilon\}] \end{aligned}$$

Next, we rewrite the delta function as a Fourier transform, $\delta(x) = \int \frac{d\alpha}{2\pi}e^{i\alpha x}$, so that $I(\epsilon,T) = I_1(\epsilon,T) + I_1(-\epsilon,T)$, where

$$I_1(\epsilon,T) = \frac{1}{2\pi}\int d\alpha d\epsilon_2 d\epsilon_3 d\epsilon_4 e^{i\alpha[\epsilon-(\epsilon_2+\epsilon_3+\epsilon_4)]}[n_2 n_3 n_4].$$

By carrying out a contour integral around the poles of the Fermi function $f(z)$ at $z = i\pi T(2n+1)$ in the lower half plane, we may deduce

$$\int_{-\infty}^{\infty} d\epsilon e^{-i(\alpha+i\delta)\epsilon} f(\epsilon) = 2\pi i T\sum_{n=0}^{\infty} e^{-(\alpha+i\delta)\pi T(2n+1)} = \frac{\pi i T}{\sinh(\alpha+i\delta)\pi T},$$

where a small imaginary part has been added to α to guarantee convergence. This enables us to carry out the energy integrals in $I_1(\epsilon,T)$, obtaining

$$I_1(\epsilon,T) = \int \frac{d\alpha}{2\pi}e^{i\alpha\epsilon}\left(\frac{\pi i T}{\sinh(\alpha+i\delta)\pi T}\right)^3$$

Now to carry out this integral, we need to distort the contour into the upper half complex plane. The function $1/\sinh(\alpha+i\delta)\pi T$ has poles at $\alpha = in/T - i\delta$, so the distorted contour wraps around the poles with $n \geq 0$. The cube of this function, has both triple and simple poles at these locations. To evaluate the residues of these poles, we expand $\sinh\alpha\pi T$ to third order in $\delta\alpha = (\alpha - \frac{in}{T})$ about the poles, to obtain

$$\sinh\alpha\pi T = (-1)^n\pi T\delta\alpha\left(1 + \frac{(\pi T)^2}{3!}\delta\alpha^2\right) + \ldots$$

So that near the poles,

$$\begin{aligned} \left(\frac{i\pi T}{\sinh\alpha\pi T}\right)^3 &= -i\frac{(-1)^n}{\delta\alpha^3}\left(1 - \frac{(\pi T)^2}{2}\delta\alpha^2\right) \\ &= -i(-1)^n\left(\frac{1}{\delta\alpha^3} - \frac{(\pi T)^2}{2\delta\alpha}\right) \end{aligned}$$

The complete contour integral becomes

$$\begin{aligned} I_1(\epsilon,T) &= \sum_{n=1}^{\infty}(-1)^n\oint\frac{d\alpha}{2\pi i}\left[\frac{1}{(\alpha-\frac{in}{T})^3} - \frac{1}{2}\frac{(\pi T)^2}{(\alpha-\frac{in}{T})}\right]e^{i\alpha\epsilon} \\ &= -\sum_{n=1}^{\infty}(-1)^n\oint\frac{d\alpha}{2\pi i}\frac{1}{(\alpha-\frac{in}{T})}\left[\frac{\epsilon^2}{2} + \frac{(\pi T)^2}{2}\right]e^{i\alpha\epsilon} \end{aligned}$$

$$= -\left[\frac{\epsilon^2}{2} + \frac{(\pi T)^2}{2}\right]\sum_{n=1}^{\infty}(-1)^n e^{-n\epsilon/T} = \frac{1}{1+e^{\epsilon/T}}\left[\frac{\epsilon^2}{2} + \frac{(\pi T)^2}{2}\right]$$

Finally, adding $I_1(\epsilon, T) + I_1(-\epsilon, T)$ finally gives

$$I(\epsilon, T) = \frac{1}{2}[\epsilon^2 + (\pi T)^2]$$

7.7.3 Kadowaki Woods Ratio and "Local Fermi Liquids"

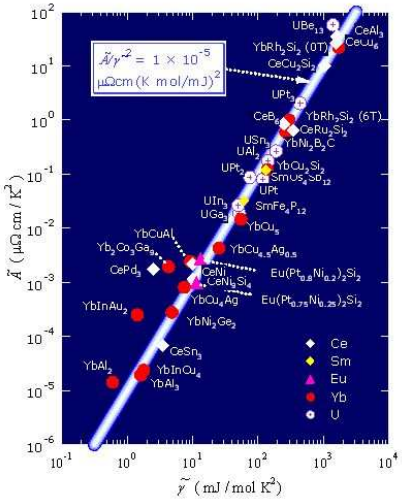


Figure 7.9: Showing the Kadowaki Woods ratio for a wide range of intermetallic "heavy electron" materials after Tsujii et al (*****).

Heuristic Discussion

One of the direct symptoms of Landau Fermi liquid behavior in a metal is a T^2 temperature dependence of resistivity at low temperatures:

$$\rho(T) = \rho_0 + AT^2.$$

Here ρ_0 is the "residual resistivity" due to the scattering of electrons off impurities. The quadratic temperature dependence in the resistivity is a direct reflection of the quadratic scattering rate $\Gamma \propto T^2$ expected in Landau Fermi liquids. Evidence that this term is directly related to electron-electron scattering is provided by a remarkable scaling relation between the A coefficient of the resistivity and the square of the zero temperature linear coefficient of the specific heat $\gamma = C_V/T|_{T\to 0}$.

$$\frac{A}{\gamma^2} = \alpha \approx 1 \times 10^{-5}\mu\Omega\text{cm(K mol/mJ)}^2$$

The ratio A/γ^2 is called the "Kadowaki Woods" ratio, and the quoted value corresponds to resistivity measured in units $\mu\Omega$cm and the specific heat coefficient per mole of material is measured in units mJ/mol/K^2. In a large large class of intermetallic metals called "heavy electron metals", in which the quasiparticle mass renormalization is particularly large, the Kadowaki Woods ratio is found to be approximately constant $\alpha = 1 \times 10^{-5}\mu\Omega$cm(K mol/mJ)^2 (Fig. 7.9).

To understand Kadowaki Woods scaling, we need to keep track of how A and γ depend on the Fermi energy. In the last section, we found that the electron-electron scattering rate is set by the Fermi energy, $\tau^{-1} \sim T^2/\epsilon_F$. If we insert this into the Drude scattering formula, for the resistivity $\rho = m^*/(ne^2\tau)$, since $m^* \propto 1/\epsilon_F$, we deduce that $\rho \sim (T^2/\epsilon_F^2)$, i.e $A \propto 1/\epsilon_F^2$. By contrast, the specific heat coefficient $\gamma \propto m^* \propto 1/\epsilon_F$, is inversely proportional to the Fermi energy, so that

$$A \propto \left(\frac{1}{\epsilon_F}\right)^2, \qquad \gamma \propto \frac{1}{\epsilon_F} \Rightarrow \frac{A}{\gamma^2} \sim \text{constant}.$$

In strongly correlated metals, the Fermi energy varies from eV to meV scales, so the A coefficient can vary over eight orders of magnitude. This strong dependence of A on the Fermi energy of the Landau Fermi liquid is cancelled by γ^2.

Estimate of the Kadowaki Woods Ratio

To obtain an estimate of the coefficient A, it is useful to regard a metal as a stack of $2D$ layers of separation a, so that $\rho = a\rho_{2D} = a/\sigma_{2D}$, where σ_{2D} is the dimensionless conductivity per layer. If we use the Drude formula for the conductivity in two dimensions $\sigma_{2D} = ne^2\tau/m$, putting $n = 2 \times \pi k_F^2/(2\pi)^2$, $\hbar/\tau = \Gamma$, we obtain

$$\rho = a \overbrace{\left(\frac{h}{2e^2}\right)}^{\rho_\square = 12.9\text{k}\Omega} \left(\frac{\Gamma}{2\epsilon_F}\right).$$

In the last section, we found that $\Gamma = 2\pi(w/4)^2(\pi k_B T)^2/\epsilon_F$. Putting this together then gives

$$\rho = (a\rho_\square)\pi\left(\frac{w}{4}\right)^2\left(\frac{\pi k_B T}{\epsilon_F}\right)^2$$

(The prefactor $a\rho_\square$ is sometimes called the "unitary resistance", and corresponds to the resistivity of a metal in which the scattering rate is of order the Fermi energy. If we put $a \sim 1-4\mathring{A}$, $\rho_\square \sim 13k\Omega$, we obtain $a\rho_\square \sim 100-500\mu\Omega cm$.) It follows that

$$A \approx (a\rho_\square)\pi^3\left(\frac{w}{4}\right)^2 \times \left(\frac{1}{T_F}\right)^2.$$

where $T_F = \epsilon_F/k_B$ is the Fermi temperature.

Now using (7.40) the specific heat coefficient per unit volume is $\gamma = \frac{1}{3}\pi^2 k_B^2 N^*(0) = \frac{\pi^2 k_B^2}{2\epsilon_F}n$, where n is the number of electrons per unit volume, thus the specific heat coefficient per electron is simply $\gamma_e = \frac{\pi^2 k_B^2}{2\epsilon_F}$ and the specific heat per mole of electrons is $\gamma_M = \frac{1}{2}\pi^2 R\frac{1}{T_F}$, where $R = k_B N_{AV}$ is the Gas constant, N_{AV} is Avagadro's number. So if there are n_e electrons per unit cell,

$$\gamma_M^2 \sim \frac{\pi^4 R^2}{4}\frac{(n_e)^2}{T_F^2} \tag{7.118}$$

giving

$$\alpha = \frac{A}{\gamma^2} \sim \left(\frac{w^2}{4\pi}\right)\left(\frac{\rho_\square}{R^2}\right) \times \frac{a}{(n_e)^2}. \tag{7.119}$$

If we take $\rho_\square = 13\times 10^9\mu\Omega$, $R = 8.3\times 10^3$mJ/mol/K and $w^2/(4\pi) \sim 1$, to obtain

$$\alpha \sim 2\times 10^{-5} \times \left(\frac{a[\text{nm}]}{(n_e)^2}\right)\mu\Omega\text{cm(K mol/mJ)}^2$$

giving a number of the right order of magnitude. Kadowaki and Woods found that $\alpha \approx 10^{-5}\mu\Omega$ cm(K mol/mJ)^2 in a wide range of intermetallic heavy fermion compounds. In transition metal compounds $\alpha \approx 0.4\times 10^{-5}\mu\Omega$cm(K mol/J)^2 has a smaller value, related to the higher carrier density.

Local Fermi Liquids

A fascinating aspect of this estimate, is that we needed to put $w^2/(4\pi) \sim 1$ to get an answer comparable with measurements. The tendency of $w \sim 1$ is a feature of a broad class of "strong correlated" metals. Although Landau Theory does not give us information on the detailed angular dependence of the scattering amplitude $A(\theta,\phi)$, we can make a great deal of progress by assuming that the scattering t-matrix is local. This is infact, a reasonable assumption in systems where the important Coulomb interactions lie within core states of an atom, as in transition metal and rare earth atoms. In this case,

$$a_{\sigma\sigma'}(\theta,\phi) = a^s + a^a\sigma\sigma'. \tag{7.120}$$

is approximately independent of the quasiparticle momenta and momentum transfer. This is the "local" approximation to the Landau Fermi liquid. When "up" quasiparticles scatter, the antisymmetry of scattering amplitudes under particle exchange guarantees that $a_{\uparrow\uparrow}(\theta,\phi) = -a_{\uparrow\uparrow}(\theta,\phi+\pi)$. But if a is independent of scattering amplitude, then it follows that $a_{\uparrow\uparrow} = a^s + a^a = 0$, so that

$$a_{\sigma\sigma'}(\theta,\phi) = a^s(1-\sigma\sigma'). \tag{7.121}$$

in a "Local" Landau Fermi liquid.

Now we can relate the $a_{\sigma\sigma'} = A_{\sigma\sigma'}/N^{*(0)}$ to the dimensionless scattering amplitudes introduced in section (7.4.3)). By (7.63), the charge susceptibility is given by

$$\chi_c = N^*(0)\times\left(\frac{1}{1+F_0^s}\right) = N^*(0)\times\left(1-\frac{F_0^s}{1+F_0^s}\right) = N^*(0)\times(1-A_0^s)$$

In strongly interacting electron systems the density of states is highly renormalized, so that $N^*(0) >> N(0)$, but the charge susceptibility is basically unaffected by interactions, given by $\chi_c = N(0) << N^*(0)$. This implies that $A_0^s \approx 1$. so that $a^s = 1/N^*(0)$, which in turn implies that the dimensionless ratio w introduced last section is close to $w = 1$.

7.8 Microscopic basis of Fermi liquid Theory

Although Landau's Fermi liquid theory is a phenomenological theory, based on physical arguments, it translates naturally into the language of diagramatic many body theory. The Landau school played a major role in the adaptation of Feynman diagramatic approaches to many body physics. However, Feynman diagrams do not appear until the third of Landau's three papers on Fermi liquid theory[**?**]. The classic microscopic treatments of Fermi liquid theory are based on the analysis of many body perturbation theory to infinite order carried out in the late 1950's and early 1960's.

Galitski[**?**], in the Soviet Union, gave the first first formulation of Landau's theory in terms of diagramatic many body theory. Shortly thereafter Luttinger, Ward and Nozieres developed the detailed diagramatic many body framework for Landau Fermi liquid theory by analysing the analytic properties of inifinite order perturbation theory[**? ?**]. Here we end with a brief discussion of some of the key results of these analyses.

From the outset, it was understood that the Landau Fermi liquid is always potentially unstable to superconductivity. By the late 1960's it also became that that Landau Fermi liquid theory does not apply in one-dimensional conductors, where the phase space scattering arguments used to support the idea of the Landau quasiparticle no longer apply. In one dimension, the Landau quasiparticle becomes unstable, breaking up into collective modes that independently carry spin and charge degrees of freedom. We call such a fluid a "Luttinger liquid". However, with this exception, few questioned the robustness of Landau Fermi liquid theory until the 1980s. In 1986, the discovery of high temperature superconductors, led to a resurgence of interest in this topic, for in the normal state, these materials can not be easily understood in terms of Landau Fermi liquid theory. For example, these materials display a linear resistivity up to high temperatures that at this time remains an unsolved mystery. This has led to the speculatation that in two or three dimensions, Landau Fermi liquid

theory might break down into a higher dimensional analog of the one-dimensional Luttinger liquid. two or even three dimensional metals. In the wake of this interest, the Landau Fermi liquid theory was re-examined from the perspective of the "renormalization group" [**?** **?**] The conclusion of these analyses is that unlike one dimension, Fermi liquids are not generically unstable in two and higher dimensions. While this does not rule the possibility of new kinds of metallic behavior, the Landau Fermi liquid theory continues to provide the bedrock for our understanding of basic metals in two or three dimensions.

As we discussed in the last chapter, the process of adiabatically "switching on" interactions can be understood as a unitary transformation of the original states of the non-interacting Fermi sea. Thus the ground state and the one-quasiparticle state are given by

$$\begin{aligned} |\phi\rangle &= U|\Psi_0\rangle, \\ |\widetilde{\mathbf{k}\sigma}\rangle &= U|\mathbf{k}\sigma\rangle \end{aligned} \tag{7.122}$$

where $|\Psi_0\rangle$ is the filled Fermi sea of the non-interacting system, and $\mathbf{k}$ is a momentum very close to the Fermi surface. In fact, using the results of (6.1), we can write U as a time-ordered exponential

$$U = T\Big[\exp\Big\{-i\int_{-\infty}^{0} V(t)dt\Big\}\Big],$$

where $\hat{V}$ is the interaction, written in the interaction representation. Now since $|\mathbf{k}\sigma\rangle = c^\dagger_{\mathbf{k}\sigma}|\Psi_0\rangle$, where $c^\dagger_{\mathbf{k}\sigma}$ is the particle creation operator for the non-interacting Hamiltonian, it follows that

$$|\widetilde{\mathbf{k}\sigma}\rangle = \overbrace{Uc^\dagger_{\mathbf{k}\sigma}U^\dagger}^{a^\dagger_{\mathbf{k}\sigma}}|\phi\rangle \tag{7.123}$$

so that the "quasiparticle creation operator" is given by

$$a^\dagger_{\mathbf{k}\sigma} = Uc^\dagger_{\mathbf{k}\sigma}U^\dagger. \tag{7.124}$$

From this line of reasoning, we can see that the operator that creates the one-quasiparticle state is nothing more than the original creation bare creation operator, unitarily time-evolved from the distant past to the present in the interaction representation.

While this formal procedure can always be carried out, the existence of the Landau Fermi liquid requires that in the thermodynamic limit, the resulting state preserves a finite overlap with the state formed by additing a bare particle to the ground-state, i.e.

$$Z_{\mathbf{k}} = |\langle\widetilde{\mathbf{k}\sigma}_0|c^\dagger_{\mathbf{k}\sigma}|\phi\rangle|^2 > 0 \qquad \text{wavefunction renormalization}$$

This overlap is called the "wavefunction renormalization constant", and so long as this quantity is finite on the Fermi surface, the Landau Fermi liquid is alive and well.

In general, near the Fermi energy, the electron creation operator will have an expansion as a sum of states containing one, three, five and any odd-number of quasiparticle and hole states, each with the same total spin, charge and momentum of the initial bare particle.

$$c^\dagger_{\mathbf{k}\sigma} = \sqrt{Z_{\mathbf{k}}}a^\dagger_{\mathbf{k}\sigma} + \sum_{\mathbf{k}_4+\mathbf{k}_3=\mathbf{k}_2+\mathbf{k}} A(\mathbf{k}_4\sigma_4, \mathbf{k}_3\sigma_3; \mathbf{k}_2\sigma_2, \mathbf{k}\sigma)a^\dagger_{\mathbf{k}_4\sigma_4}a^\dagger_{\mathbf{k}_3\sigma_3}a_{\mathbf{k}_2\sigma_2} + \ldots$$

There are three important consequences that follow from this result:

- **Sharp Quasiparticle peak in the spectral function.**

  When a particle is added to the ground-state, it excites a continuum of states $|\lambda\rangle$, with energy distribution described by the spectral function (7.112),

  $$A(\mathbf{k},\omega) = \frac{1}{\pi}\mathrm{Im}G(\mathbf{k},\omega - i\delta) = \sum_\lambda |M_\lambda|^2\delta(\omega-\epsilon_\lambda). \tag{7.125}$$

  where the squared amplitude $|M_\lambda|^2 = |\langle\lambda|c^\dagger_{\mathbf{k}\sigma}|\phi\rangle|^2$. In a Landau Fermi liquid, the spectral function retains a sharp "quasiparticle pole" at the Fermi energy. If we split off the $\lambda \equiv \mathbf{k}\sigma$ contribution to the summation in (7.125) we then get

  $$A(\mathbf{k},\omega) = \frac{1}{\pi}\mathrm{Im}G(\mathbf{k},\omega-i\delta) = \overbrace{Z_{\mathbf{k}\sigma}\delta(\omega-\epsilon_{\mathbf{k}})}^{\text{qp peak}} + \overbrace{\sum_{\lambda\neq\mathbf{k}\sigma}|M_\lambda|^2\delta(\omega-\epsilon_\lambda)}^{\text{continuum}}. \tag{7.126}$$

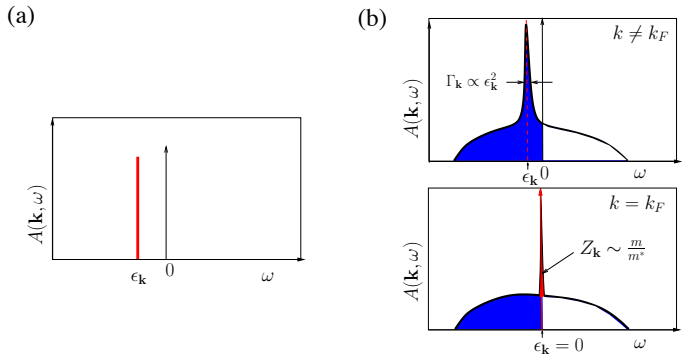


Figure 7.10: (a) In a non-interacting Fermi system, the spectral function is a sharp delta function at $\omega = \epsilon_{\mathbf{k}}$. (b) In an interacting Fermi liquid for $k \neq k_F$, the quasiparticle forms a broadened peak of width $\Gamma_{\mathbf{k}}$ at $\omega_{\mathbf{k}}$. If $k = k_F$, this peak becomes infinitely sharp, corresponding to a long-lived quasiparticle on the Fermi surface. The weight in the quasiparticle peak is $Z_{\mathbf{k}} \sim m/m^*$, where m^* is the effective mass.

- **Sudden jump in the momentum distribution.**

In a non-interacting Fermi liquid, the particle momentum distribution function exhibits a sharp Fermi distribution function which is preserved by the *quasiparticles* in a Landau Fermi liquid theory

$$\langle\phi|(\hat{n}_{\mathbf{k}\sigma})_{\rm qp}|\phi\rangle = \theta(\mu - E_{\mathbf{k}})$$

where here $(\hat{n}_{\mathbf{k}\sigma})_{\rm qp} = \tilde{c}^{\dagger}_{\mathbf{k}\sigma}\tilde{c}_{\mathbf{k}\sigma}$ is the quasiparticle occupancy. Remarkably, part of this jump survives interactions. To see this effect, we write the momentum distribution function of the particles as

$$\langle\hat{n}_{\mathbf{k}\sigma}\rangle = \langle\phi|c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|\phi\rangle = \int_{-\infty}^{0} d\omega A(\mathbf{k},\omega)$$

where we have used the results of (6.3.3) to relate the particle number to the integral over the spectral function below the Fermi energy. When we insert (7.126) into this expression, the contribution from the quasiparticle peak vanishes if $\epsilon_{\mathbf{k}} > 0$, but gives a contribution $Z_{\mathbf{k}}$ if $\epsilon_{\mathbf{k}} < 0$, so that

$$\langle\hat{n}_{\mathbf{k}\sigma}\rangle = Z_{\mathbf{k}}\theta(-\epsilon_{\mathbf{k}}) + \text{smooth background.}$$

This is a wonderful illustration of the organizing power of the Pauli exclusion principle. One might have expected interactions to have the same effect as temperature which smears the Fermi distribution by an amount of order k_BT. Although interactions do smear the momentum distribution, the jump continues to survive in reduced form so long as the Landau Fermi liquid is intact.

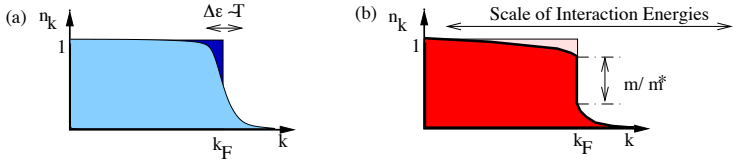


Figure 7.11: (a) In a non-interacting Fermi liquid, a temperature T that is smaller than the Fermi energy, slightly "blurs" the Fermi surface; (b) In a Landau Fermi liquid, the exclusion principle stabilizes the jump in occupancy at the Fermi surface, even though the bare interaction energy is far greater than than the Fermi energy,

- **Luttinger sum rule**.

  In the Landau Fermi liquid, the Fermi surface volume measures the particle density n_F. Since the Fermi surface of the quasiparticles and the unrenormalized particles coincides, it follows that the Fermi surface volume must be an adiabatic invariant when the interactions are turned on.

$$n_F = (2S+1)\frac{v_{\rm FS}}{(2\pi)^3}, \qquad \text{(Luttinger sum rule)}$$

  The demonstration of this conservation law within infinite order perturbation theory was first derived by Luttinger in 1962, and is known as the Luttinger sum rule. In interacting fermion

systems the conservation of particle number leads to a set of identities between different many body Greens functions called "Ward Identities". Luttinger showed how these identities can be used to relate the Fermi surface volume to the particle density.

Today, more than a half century after Landau's original idea, the Landau Fermi liquid theory continues to be a main-stay of our understanding of interacting metals. However, increasingly, physicists are questioning when and how, does the Landau Fermi liquid break-down, and what new types of fermion fluid may form instead? We know that Landau Fermi liquid does not survive in one-dimensional conductors, where quasiparticles break up into collective spin and charge excitations. or in high magnetic fields where the formation of widely spaced Landau levels effectively quenches the kinetic energy of the particles, enhancing the relative importance of interactions. In both these examples, new kinds of quasiparticle description are required to describe the physics. Today, experiments strongly suggest indication that the Landau Fermi liquid breaks up into new kinds of "Non-Fermi liquid" fluid at a zero temperature phase transition, or quantum critical point, giving rise to new kinds of metallic behavior in electron systems. The quest to understand these new metals and to characterize their excitation spectrum is one of the great open problems of modern condensed matter theory.

Chapter 8

Feynman Diagrams: T=0

Chapter 6. discussed adiabaticity, and we learned how Green's functions of an interacting system, can be written in terms Green's functions of the non-interacting system, weighted by the S-matrix, e.g.

$$\langle\phi|T\psi(1)\psi^\dagger(2)|\phi\rangle = \frac{\langle\phi_o|T\hat{S}\psi(1)\psi^\dagger(2)|\phi_o\rangle}{\langle\phi_o|\hat{S}|\phi_o\rangle}$$

$$\hat{S} = T\exp\Big[-i\int_{-\infty}^{\infty}V(t')dt'\Big] \tag{8.1}$$

where $|\phi_o\rangle$ is the ground-state of H_o. In chapter 7. we showed how the concept of adiabaticity was used to establish Landau Fermi liquid theory. Now we move on to will learn how to expand the fermion Green's function and other related quantities order by order in the strength of the interaction. The Feynman diagram approach, originally developed by Richard Feynman to describe the many body physics of quantum electrodynamics[1], and later cast into a rigorous mathematical framework by Freeman Dyson, [2] provides a succinct visual rendition of this expansion, a kind of **"mathematical impressionism"** which is physically intuitive, without losing mathematical detail.

From the Feynman rules, we learn how to evaluate

- The ground-state $S-$ matrix

$$S = \langle\phi_o|\hat{S}|\phi_o\rangle = \sum\{\text{Unlinked Feynman Diagrams}\}. \tag{8.2}$$

- The logarithm of the $S-$ matrix, which is directly related to the shift in the ground-state energy due to interactions.

$$E - E_o = \lim_{\tau\to\infty}\frac{\partial}{\partial\tau}\ln\langle\phi_o|S[\tau/2,-\tau/2]|\phi_o\rangle = i\sum\{\text{Linked Feynman Diagrams}\} \tag{8.3}$$

where each Linked Feynman diagrams describes a different virtual excitation.

- Green's functions.

$$G(1-2) = \sum\{\text{Two-legged Feynman Diagrams}\} \tag{8.4}$$

- Response functions. These are a different type of Green's function, of the form

$$\mathcal{R}(1-2) = -i\langle\phi|[A(1),B(2)]|\phi\rangle\theta(t_1-t_2) \tag{8.5}$$

8.1 Heuristic Derivation

Feynman initially derived his diagramatic expansion as a mnemonic device for calculating scattering amplitudes. His approach was heuristic: each diagram has a physical meaning in terms of a specific scattering process. Feynman derived a set of rules that explained *how* to convert the diagrams into concrete scattering amplitudes. These rules were fine tuned and tested in the simple cases where they could be checked by other means; later, he applied his method to cases where the direct algebraic approach was impossibly cumbersome. Later, Dyson gave his diagramatic expansion a systematic mathematical framework.

Learning Feynman diagrams is a little like learning a language. You can learn the rules, and work by the book, but to really understand it, you have to work with it, gaining experience in practical situations, learning it not just as a theoretical construct, but as a living tool to communicate ideas. One can be a beginner or an expert, but to make it work for you, like a language or a culture, you will have to fall in love with it!

Formally, a perturbation theory for the fully interacting S-matrix is obtained by expanding the S-matrix as a power-series, then using Wick's theorem to write the resulting correlation functions as a sum of contractions.

$$\langle\phi_o|\hat{S}|\phi_o\rangle = \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}dt_1\ldots dt_n\sum_{\text{Contractions}}\langle\phi_o|T\,\overbrace{V(t_1)V(t_2)\ldots V(t_n)}\,|\phi_o\rangle \tag{8.6}$$

The Feynman rules tell us how to expand these contractions as a sum of diagrams, where each diagram provides a precise, graphical representation of a scattering amplitude that contributes to the complete S-matrix.

Let us see examine how we might develop, heuristically, a Feynman diagram exapnsion for simple potential scattering, for which

$$V(1) \equiv \int d^3x_1 U(\vec{x}_1)\psi^\dagger(\vec{x}_1,t_1)\psi(\vec{x}_1,t_1). \tag{8.7}$$

where we've suppressed spin indices into the background. When we start to make contractions we will break up each product $V(1)V(2)\ldots V(r)$ into pairs of creation and annihilation operators, replacing each pair as follows

$$\overbrace{\psi(2)\ldots\psi^\dagger(1)} \;\to\; (\sqrt{i})^2\times G(2-1). \tag{8.8}$$

where we have divided up the the prefactor of i two factors of $\sqrt{i}$, which we will transfer onto the scattering amplitudes where the particles are created and annihilated. This contraction is denoted by

$$G(2-1) = 2 \longleftarrow 1 \tag{8.9}$$

representing the propagation of a particle from "1" to "2". Pure potential scattering gives us one incoming, and one outgoing propagator, so we denote a single potential scattering event by the diagram

$$\sqrt{i},\ \sqrt{i},\ -iU(x) \qquad = (\sqrt{i})^2 \times -iU(x) \equiv U(x) \tag{8.10}$$

Here, the "$-i$" has been combined with the two factors of $\sqrt{i}$ taken from the incoming, and outgoing propagators to produce a purel *real* scattering amplitude $(\sqrt{i})^2 \times -iU(x) = U(x)$.

The Feynman rules for pure potential scattering tell us that the S-matrix for potential scattering is the exponential of a sum of connected "vacuum" diagrams

$$S = \exp[\ \bigcirc + \bigcirc\!\!\bullet\!\!\bigcirc + \bigcirc\!\!\bullet\!\!\bigcirc\!\!\bullet\!\!\bigcirc + \ldots\ ]\,. \tag{8.11}$$

The "vacuum diagrams" appearing in the exponential do not have any incoming or outgoing propagators- they represent the amplitudes for the various possible processes by which electron-hole pairs can bubble out of the vacuum. Let us examine the first, and second order contractions for potential scattering. To first order

$$-i\langle\phi_0|\overbrace{V(t_1)}\ |\phi_0\rangle \;=\; -i\sum_\sigma \int d^3x U(x)\langle\phi_0|T\,\overbrace{\psi^\dagger_\sigma(x,t_1^+)\psi_\sigma(x,t_1^-)}\ |\phi_0\rangle \tag{8.12}$$

This contraction describes a single scattering event at $(\vec{x}, t_1)$. Note that the creation operator occurs to the *left* of the annihilation operator, and to preserve this ordering inside the time-ordered exponential, we say that the particle propagates "backwards in time" from $t = t_1^+$ to $t = t_1^-$. When we replace this term by a propagator the backward time propagation introduces a factor of $\zeta = -1$ for fermions, so that

$$\langle\phi_0|T\,\overbrace{\psi^\dagger_\sigma(x,t_1^+)\psi_\sigma(x,t_1^-)}\ |\phi_0\rangle = i\zeta G(\vec{x}-\vec{x}, t_1^- - t_1^+) = i\zeta G(\vec{0}, 0^-) \tag{8.13}$$

We carry along the factor $U(\vec{x})$ as the amplitude for this scattering event. The result of this contraction procedure is then

$$-i\int_{-\infty}^{\infty} dt_1\langle\phi_0|\overbrace{V(t_1)}\ |\phi_0\rangle \;=\; -i(2S+1)\int dt_1 \times \int d^3x U(x) \times i\zeta G(\vec{0}, 0^-)$$
$$= \quad \bigcirc, \tag{8.14}$$

where we have translated the scattering amplitude into a a single diagram. You can think of it as the spontaneous creation, and re-annhilation of a single particle. Here we may tentatively infer a number of important "Feynman rules" - listed in Table 8.1: that we must associate each scattering event with an amplitude $U(x)$, connected by propagators that describe the amplitude for electron motion between scattering events. The overall amplitude involves an integration over the space time co-ordinates of the scattering events, and apparently, when a particle loop appears, we need to introduce the factor $\zeta(2S+1)$ (where $\zeta = -1$ for fermions) into the scattering amplitude to account for the presence of an odd-number of backwards-time propagators and the $2S+1$ spin components of the particle field. These rules are summarized in the table below:

Physically, the vacuum diagram we have drawn here can be associated with the small first-order shift in the energy ΔE_1 of the particle due to the potential scattering. This inturn produces a phase shift in the scattering S-matrix,

$$S \sim \exp\left[-i\Delta E_1 \int dt\right] \sim 1 - i\Delta E_1 \int dt, \tag{8.15}$$

where the exponential has been audaciously expanded to linear order in the strength of the scattering potential. If we compare this result with our leading Feynman diagram expansion of the S-matrix,

$$\langle\phi_o|\hat{S}|\phi_o\rangle = 1 + \bigcirc,$$

we see that we can interpret the overall factor of $\int dt_1$ in (8.14) as the time period over which the scattering potential acts on the particle. If we factor this term out of the expression we may identify

$$\Delta E_1 = \overbrace{i\zeta(2S+1)G(\vec{0}, 0^-)}^{\rho} \int d^3x U(x) \tag{8.16}$$

Here, following our work in the previous chapter, we have identified $i\zeta(2S+1)G(\vec{0}, 0^-) = \sum_\sigma \langle\psi^\dagger{}_\sigma(x)\psi_\sigma(x)\rangle = \rho$ as the density of particles. giving $\Delta E_1 = \rho\int d^3x U(x)$. The correspondence of our result with first order perturbation theory is a check that the tentative Feynman rules are correct.

Let us go on to look at the second order contractions

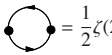
$$\langle\phi_0|TV(t_1)V(t_2)\ |\phi_0\rangle \;=\; \langle\phi_0|T\overbrace{V(t_1)}\overbrace{V(t_2)}\ |\phi_0\rangle + \langle\phi_0|T\,\overbrace{\overbrace{V(t_1)}V(t_2)}\ |\phi_0\rangle \tag{8.17}$$

which now generate two diagrams

$$\frac{1}{2!}(-i)^2\int_{-\infty}^{\infty} dt_1 dt_2\langle\phi_0|T\ \overbrace{V(t_1)}\overbrace{V(t_2)}\ |\phi_0\rangle \;=\; \frac{1}{2}\left[\ \bigcirc\ \right]^2 = \left[\ \bigcirc\ \bigcirc\ \right]$$

$$\frac{1}{2!}(-i)^2\int_{-\infty}^{\infty}dt_1dt_2\langle\phi_0|T\,\overbrace{V(t_1)V(t_2)}\,|\phi_0\rangle \quad = \quad$$  (8.18)

The first term is simply a product of two first order terms- the beginning of an exponential combination of such terms. Notice how the square of one diagram is the original diagram, repeated twice. The factor of $1/2$ that occurs in the expression on the left hand-side is absorbed into this double diagram as a so-called "symmetry factor". We shall return to this issue shortly, but briefly, this diagram has a permutation symmetry described by a group of dimension $d = 2$, according to the Feynman rules, this generates a prefactor $1/d = 1/2$. The second term derives from the second-order shift in the particle energies due to scattering, and which, like the first order shift, produces a phase shift in the S-matrix. This diagram has a cyclic group symmetry of dimension $d = 2$, and once again, there is a symmetry factor of $1/d = 1/2$. This connected, second-order diagram gives rise to the scattering amplitude

 $= \frac{1}{2}\zeta(2S+1)\int d1d2U(1)U(2)G(1-2)G(2-1)$ (8.19)

where $1 \equiv (\vec{x_1}, t_1)$, so that

$$\begin{aligned}\int d1 &\equiv \int dt_1 d^3x_1\\ G(2-1) &\equiv G(\vec{x}_2-\vec{x_1}, t_2-t_1).\end{aligned} \tag{8.20}$$

Once again, the particle loop gives a factor $\zeta(2S+1)$, and the amplitude involves an integral over all possible space-time co-ordinates of the two scattering events. You may interpret this diagram in various ways- as the creation of a particle-hole pair at $(\vec{x_1}, t_1)$ and their subsequent reannilation at $(\vec{x}_2, t_2)$ (or vice versa). Alternatively, we can adopt an idea that Feynman developed as a graduate student with John Wheeler- the idea than that an anti-particle (or hole), is a particle propagating backwards in time. From this perspective, this second-order diagram represents a *single* particle that propagates around a loop in space time. Equation (8.19) can be simplified by first making the change of variables $t = t_1 - t_2$, $T = (t_1 + t_2)/2$, so that $\int dt_1dt_2 = \int dT \times \int dt$. Next, if we Fourier transform the scattering potential and Green functions, we obtain

 $= \int dT \times \frac{1}{2}\zeta(2S+1)\int dtd^3qd^3k|U(\vec{q}_1)|^2G(\vec{k}+\vec{q},t)G(\vec{k},-t)$ (8.21)

Once again, an overall time-integral factors out of the overall expression, and we can identify the remaining term as the *second-order* shift in the energy

$$\Delta E_2 = \frac{i}{2}\zeta(2S+1)\int dt\frac{d^3k}{(2\pi)^3}\frac{d^3q}{(2\pi)^3}|U(\vec{q}_1)|^2G(\vec{k}+\vec{q},t)G(\vec{k},-t). \tag{8.22}$$

To check that this result is correct, let us consider the case of fermions, where

$$G(\mathbf{k},t) = -i[(1-n_{\mathbf{k}})\theta(t) - n_{\mathbf{k}}\theta(-t)]e^{-i\epsilon_{\mathbf{k}}t} \tag{8.23}$$

which enables us to do the integral

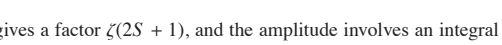
$$i\int dte^{-\delta|t|}G(\vec{k}+\vec{q},t)G(\vec{k},-t) \quad = \quad \frac{(1-n_{\mathbf{k+q}})n_{\mathbf{k}}}{\epsilon_{\mathbf{k+q}}-\epsilon_{\mathbf{k}}} + (\mathbf{k}\leftrightarrow\mathbf{k}+\mathbf{q}) \tag{8.24}$$

We recognize the first process as the virtual creation of an electron of momentum $\vec{k}+\vec{q}$, leaving behind a hole in the state with momentum $\vec{k}$. The second-term is simply a duplicate of the first, with the momenta interchanged, and the sum of the two terms cancels the factor of $1/2$ infront of the integral. The final result

$$\Delta E_2 = -(2S+1)\int\frac{d^3k}{(2\pi)^3}\frac{d^3q}{(2\pi)^3}|U(\vec{q})|^2\frac{(1-n_{\mathbf{k+q}})n_{\mathbf{k}}}{\epsilon_{\mathbf{k+q}}-\epsilon_{\mathbf{k}}}$$

is recognized as the second-order correction to the energy derived from these virtual processes. Of course, we could have derived these results directly, but the important point, is that we have established a tentative link between the diagramatic expansion of the contractions, and the perturbation expansion for the ground-state energy. Moreover, we begin to see that our diagrams have a direct interpretation in terms of the virtual excitation processes that are generated by the scattering events.

To second-order, our results do indeed correspond to the leading order terms in the exponential

$S = 1 +$  $+ \frac{1}{2!}\Big[$ $+\ldots\Big]^2 + \cdots = exp\Big[$ $+\ldots\Big]$.

Before we go on to complete this connection more formally in the next section, we need to briefly discuss "source terms", which couple directly to the creation and annihilation operators. The source terms let us examine how the S-matrix responds to incoming currents of particles. Source terms add directly to the scattering potential, so that

$$V(1) \longrightarrow V(1) + \bar{\eta}(1)\psi(1) + \psi^\dagger(1)\eta(1).$$

The source terms involve a single creation or annihilation operator, thus produce either the beginning

 $\eta(1) \equiv \int d1\cdots\times\eta(1)$ (8.25)

or the end

$-i\bar{\eta}$ $\equiv -i\int d2\bar{\eta}(2)\times\ldots$ (8.26)

of a Feynman diagram. In practice, each $\bar{\eta}$ and η arrive in pairs, and the factor $-i$ which multiplies $\bar{\eta}$ combines the two factors of $-i$ from a pair $(\bar{\eta}, \eta)$ with the factor of i derived from the propagator

line they share. We need these terms, so that we can generate diagrams which involve incoming and outgoing electrons. The simplest contraction with these terms generates the bare propagator

$$\begin{aligned}
&\frac{(-i)^2}{2!}\int d2d1\langle 0|\Big[V(2)+\bar\eta(2)\overbrace{\psi(2)+\bar\psi^\dagger(2)\eta(2)}\Big]\Big[V(1)+\bar\eta(1)\overbrace{\psi(1)+\bar\psi^\dagger(1)\eta(1)}\Big]|0\rangle\\
&= \int d1d2\Big(\sqrt{-i}\bar\eta(2)G(2-1)\sqrt{-i}\eta(1)\Big)\\
&= -i\bar\eta\longleftarrow\eta. \qquad (8.27)
\end{aligned}$$

If we now include the contraction with the first scattering term we produce the first scattering correction to the propagator

$$\begin{aligned}
&\frac{(-i)^3}{3!}\int d2dXd1\langle 0|\Big\{[\ldots+\bar\eta(2)\overbrace{\psi(2)+\ldots]\Big[U(X)\bar\psi^\dagger(X)}\overbrace{\psi(X)+\ldots\Big]\Big[\ldots+\bar\psi^\dagger(1)\eta(1)\Big]}+\text{perms}\Big\}|0\rangle\\
&\qquad = \int d1d2\Big(\sqrt{-i}\bar\eta(2)\int dXG(2-X)V(X)G(X-1)\sqrt{-i}\eta(1)\Big)\\
&\qquad = -i\eta\longleftarrow\bullet\longleftarrow\eta. \qquad (8.28)
\end{aligned}$$

where we have only shown one of *six* equivalent contractions on the first line. This diagram is simply interpreted as a particle, created at 1, scattering at position X before propagating onwards to position 2. Notice how we must integrate over the the space-time co-ordinate of the intermediate scattering event at X, to obtain the total first order scattering amplitude. Higher order corrections will merely generate multiple insertions into the propagator and we will have to integrate over the space-time co-ordinate of each of these scattering events. Diagramatically, the sum over all such diagrams generates the "renormalized propagator", denoted by

$G^*(2-1) = 2 \Longleftarrow 1$

$= 2 \longleftarrow 1 + 2 \longleftarrow 1 + 2 \longleftarrow 1 + \ldots$ (8.29)

Indeed, to second-order in the scattering potential, we can see that all the allowed contractions are consistent with the following exponential form for the generating functional

$S = exp\Big[$ + + $\cdots - i\bar\eta\Longleftarrow\eta\Big]$. (8.30)

To prove this result formally requires a little more work, that we now go into in more detail. The important point for you to grasp right now, is that the sum over all contractions in the S-matrix can be represented by a sum of diagrams which concisely represent the contributions to the scattering amplitude as a sum over all possible virtual excitation processes about the vacuum.

8.2 Developing the Feynman Diagram Expansion

A neat way to organize this expansion is obtained using the source term approach we encountered in the last chapter. There we found we could completely evaluate the the response of a non-interacting the system to a source term which injected and removed particles. We start with the source term S-matrix

$$\hat S[\bar\eta,\eta] = T\exp\Big[-i\int d1[\psi^\dagger(1)\eta(1)+\bar\eta(1)\psi(1)]\Big]. \qquad (8.31)$$

Here, for convenience, we shall hide details of the spin away with the space-time co-ordinate, so that $1\equiv(\mathbf{x}_1,t_1,\sigma_1)$, $\psi(1)\equiv\psi_\sigma(\mathbf{x},t)$. You can think of the quantities $\eta(1)$ and $\bar\eta(1)$ as "control-knobs" which we dial up, or down, the rate at which we are adding, or subtracting particles to the system. For fermions, these numbers must be anticommuting Grassman numbers: numbers which anticommute with each and all Fermion field operators. The vacuum expectation value of this S-matrix is then

$$S[\bar\eta,\eta] = \langle\phi|\hat S[\bar\eta,\eta]|\phi\rangle = \exp\Big[-i\int d1d2\bar\eta(1)G(1-2)\eta(2)\Big] \qquad (8.32)$$

where here, $G(1-2)\equiv\delta_{\sigma\sigma_2}G(\mathbf{x}_1-\mathbf{x}_2,t_1-t_2)$ is diagonal in spin. In preparation for our diagramatic approach, we shall denote

$$\int d1d2\bar\eta(1)G(1-2)\eta(2) = \bar\eta\longleftarrow\eta \qquad (8.33)$$

where an integral over the space-time variables $(\mathbf{x}_1,t_1)$ and $(\mathbf{x}_2,t_2)$ and a sum over spin variables σ_1, σ_2 is implied by the diagram. The S-matrix equation can then be written

$$S[\bar\eta,\eta] = \exp\Big[-i\bar\eta\longleftarrow\eta\Big] \qquad (8.34)$$

This is called a "generating functional". By differentiating this quantity with respect to the source terms, we can compute the expectation value of any product of operators. Grassman numbers and their differential operators anticommute with each other, and with the field operators. [1] Each time we differentiate the S-matrix with respect to $\bar\eta(1)$, we pull down a field operator inside the time-ordered product

$$\begin{aligned}
i\frac{\delta}{\delta\bar\eta(1)} &\rightarrow \psi(1)\\
i\frac{\delta}{\delta\bar\eta(1)}\langle\phi|T\hat S\{\ldots\}|\phi\rangle &= \langle\phi|T\hat S\{\ldots\psi(1)\ldots\}|\phi\rangle \qquad (8.35)
\end{aligned}$$

[1] For example, if $F[\bar\eta,\eta] = \bar A\eta+\bar\eta A+B\bar\eta\eta$, where A, $\bar A$, η and $\bar\eta$ are Grassman numbers, while B is a commuting number, then $\frac{\partial F}{\partial\bar\eta} = A+B\eta$, but $\frac{\partial F}{\partial\eta} = -\bar A-B\bar\eta$ because the differential operator anticommutes with $\bar A$ and $\bar\eta$. The second derivative $\frac{\partial^2 F}{\partial\eta\partial\bar\eta} = -\frac{\partial^2 F}{\partial\bar\eta\partial\eta} = B$, illustrating that the differential operators of Grassman numbers anticommute.

For example, the field operator has an expectation value

$$\begin{aligned}\langle\psi(1)\rangle &= \frac{\langle\phi|\hat{S}[\bar{\eta},\eta]\psi(1)|\phi\rangle}{\langle\phi|\hat{S}[\bar{\eta},\eta]|\phi\rangle} = i\frac{\delta}{\delta\bar{\eta}(1)}\ln S[\bar{\eta},\eta]\\ &= \int G(1-2)\eta(2)d2\\ &\equiv [1 \longleftarrow \eta] \end{aligned} \tag{8.36}$$

Notice how the differential operator $i\frac{\delta}{\delta\bar{\eta}(1)}$ "grabs hold" of the end of a propagator and connects it up to space-time co-ordinate 1. Likewise, each time we differentiate the S-matrix with respect to $\eta(1)$, we pull down a field creation operator inside the time-ordered product.

$$i\zeta\frac{\delta}{\delta\eta(1)} \to \psi^\dagger(1), \tag{8.37}$$

The appearance of a "ζ" in (8.37) compared with the "$+i$" in (8.35) arises because the source term anticommutes with the field operators, $\psi^\dagger(1)\eta(1) = -\eta(1)\psi^\dagger(1)$, so that

$$\frac{\delta}{\delta\eta(1)}\int dX\psi^\dagger(X)\eta(X) = \zeta\frac{\delta}{\delta\eta(1)}\int dX\eta(X)\psi^\dagger(X) = \zeta\psi^\dagger(1) \tag{8.38}$$

and the expectation value of the creation operator has the value

$$\begin{aligned}\langle\psi^\dagger(2)\rangle &= \frac{\langle\phi|\hat{S}[\bar{\eta},\eta]\psi^\dagger(2)|\phi\rangle}{\langle\phi|\hat{S}[\bar{\eta},\eta]|\phi\rangle} = i\zeta\frac{\delta}{\delta\eta(2)}\ln S[\bar{\eta},\eta]\\ &= \int d1\bar{\eta}(1)G(1-2)\\ &\equiv [\bar{\eta} \longleftarrow 2] \end{aligned} \tag{8.39}$$

If we differentiate either (8.36) w.r.t. $\eta(2)$, or (8.39) w.r.t. $\bar{\eta}(1)$ we obtain

$$\frac{\delta}{\delta\eta(2)}\langle\psi(1)\rangle\Big|_{\eta=\bar{\eta}=0} = \frac{\delta}{\delta\bar{\eta}(1)}\langle\psi^\dagger(2)\rangle\Big|_{\eta=\bar{\eta}=0} = -i\langle\phi|T\psi(1)\psi^\dagger(2)|\phi\rangle = G(1-2) \tag{8.40}$$

as expected.

In general, we can calculate arbitrary functions of the field operators by acting on the S-matrix with the appropriate function of derivative operators.

$$\langle\phi|T\hat{S}[\bar{\eta},\eta]F[\psi^\dagger,\psi]|\phi\rangle = F\Big[i\zeta\frac{\delta}{\delta\eta}, i\frac{\delta}{\delta\bar{\eta}}\Big]\exp\Big[-i\bar{\eta} \longleftarrow \eta\Big]. \tag{8.41}$$

If we now set $F[\psi^\dagger,\psi] = Te^{-i\int V[\psi^\dagger,\psi]dt}$, then

$$S_I[\bar{\eta},\eta] = \langle\phi|Te^{-i\int_{-\infty}^{\infty}dt\left(V(\psi^\dagger,\psi)+\text{source terms}\right)}|\phi\rangle \tag{8.42}$$

can be written completely algebraically, in the form

$$S_I[\bar{\eta},\eta] = e^{-i\int_{-\infty}^{\infty}V(i\zeta\frac{\delta}{\delta\eta},i\frac{\delta}{\delta\bar{\eta}})dt}\exp\Big[-i\bar{\eta} \longleftarrow \eta\Big] \tag{8.43}$$

The action of the exponentiated differential operator on the source terms generates all of the contractions. It is convenient to recast this expression in a form that groups all the factors of "i". To do this, we write $\alpha = \eta, \bar{\alpha} = -i\bar{\eta}$, this enables us to rewrite the expression as $S_I[\bar{\eta},\eta] = \mathcal{S}_I[\bar{\alpha},\alpha]|_{\alpha=\eta,\bar{\alpha}=-i\bar{\eta}}$, where

$$\mathcal{S}_I[\bar{\alpha},\alpha] = e^{(i)^{n-1}\int_{-\infty}^{\infty}V(\zeta\frac{\delta}{\delta\alpha},\frac{\delta}{\delta\bar{\alpha}})dt}\exp\Big[\bar{\alpha} \longleftarrow \alpha\Big]$$

where we have written

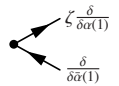
$$V(i\zeta\frac{\delta}{\delta\eta}, i\frac{\delta}{\delta\bar{\eta}}) = i^nV(\zeta\frac{\delta}{\delta\alpha},\frac{\delta}{\delta\bar{\alpha}}) \tag{8.44}$$

for an interaction involving n creation and n annihilation operators (n-particle interaction). This equation provides the basis for all Feynman diagram expansions.

To develop the Feynman expansion, we need to recast our expression in a more graphical form. To see how this works, let us first consider a one-particle scattering potential ($n = 1$). In this case, we write

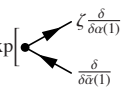
$$i^{n-1}V(\zeta\frac{\delta}{\delta\alpha},\frac{\delta}{\delta\bar{\alpha}}) = \int d^3xU(x)\Big(\zeta\frac{\delta}{\delta\alpha(x)}\frac{\delta}{\delta\bar{\alpha}(x)}\Big) \tag{8.45}$$

which we denote as

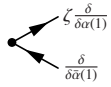


(8.46)

Notice that the basic scattering amplitude for scattering at point x is simply $U(x)$ (or $U(x)/\hbar$ if we reinstate Planck's constant). Schematically then, our Feynman diagram expansion can be written as

$$\mathcal{S}_I[\bar{\alpha},\alpha] = \exp\Big[$$  $$\Big]\exp\Big[\bar{\alpha} \longleftarrow \alpha\Big]$$

The differential operators acting on the bare S-matrix, glue the scattering vertices to the ends of the propagators, and thereby generate a sum of all possible Feynman diagrams. Formally, we must expand the exponentials on both sides, e.g.

$$\mathcal{S}_I[\bar{\alpha},\alpha] = \sum_{n,m}\frac{1}{n!m!}\Big[$$  $$\Big]^n\Big[\bar{\alpha} \longleftarrow \alpha\Big]^m \tag{8.47}$$

The action of the differential operator on the left hand-side is to glue the m propagators together with the n vertices, to make a series of Feynman diagrams. Now, at first sight, this sounds pretty frightening- we will have a profusion of diagrams. Let us just look at a few: do not at this stage worry about the details, just try to get a feeling for the general structure. The simplest $n = 1, m = 1$ term takes the form

$$\Big[\ \zeta\tfrac{\delta}{\delta\alpha(1)}\ ,\ \tfrac{\delta}{\delta\bar\alpha(1)}\ \Big]\Big[\bar\alpha \longleftarrow \alpha\Big] = \zeta\int d1V(1)\frac{\delta^2}{\delta\alpha(1)\delta\bar\alpha(1)}\int dXdY\bar\alpha(X)G(X-Y)\alpha(Y)$$
$$= \zeta\int d1V(1)G(1^- - 1) = \qquad (8.48)$$

This is the simplest example of a "linked-cluster" diagram, and it results from a single contraction of the scattering potential. The sign $\zeta = -1$ occurs for fermions, because the fermi operators need to be interchanged to write the expression as a time-ordered propagator. One can say that the expectation value involves the fermion propagating backwards in time from time t to an infinitesimally earlier time $t^- = t - \epsilon$. The term $n = 1, m = 2$ gives rise to two sets of diagrams, as follows:

$$\Big[\ \zeta\tfrac{\delta}{\delta\alpha(1)}\ ,\ \tfrac{\delta}{\delta\bar\alpha(1)}\ \Big]\Big[\bar\alpha \longleftarrow \alpha\Big]^2 = \bar\alpha \longleftarrow\!\bullet\!\longleftarrow \alpha + [\ \times\ \bar\alpha \longleftarrow \alpha] \qquad (8.49)$$

The first term corresponds to the first scattering correction to the propagator, written out algebraically,

$$\bar\alpha \longleftarrow\!\bullet\!\longleftarrow \alpha = \int d1d2\bar\alpha(1)\int dXG(1-X)V(X)G(X-2)\alpha(2)$$

whereas the second term is an unlinked product of the bare propagator, and the first linked cluster diagram. The Feyman rules enable us to write each possible term in the expansion of the S-matrix as a sum of unlinked diagrams. Fortunately, we are able to systematically combine all of these diagrams together, with the end result that

$$S_I(\bar\alpha,\alpha) = \exp\Big[\sum \text{linked diagrams}\Big]$$
$$= exp\Big[\ \ +\ \ +\ \ldots\ \bar\alpha \Longleftarrow \alpha\Big]. \qquad (8.50)$$

When written in this exponential form, the unlinked diagrams entirely disappear- a result of the so-called "link-cluster" theorem we are shortly to encounter. The Feynman rules tell us how to convert these diagrams into mathematical expressions. These rules are summarized in table 8.1.

Let us now look at how the same procedure works for a two-particle interaction. Working heuristically, we expect a two-body interaction to involve two incoming and two outgoing propagators. We shall denote a two-body scattering amplitude by the following diagram

$$\mathbf{1}\ \ \mathbf{2} = (\sqrt{i})^4 \times -iV(1-2) \equiv iV(1-2). \qquad (8.51)$$

Notice how, in contrast to the one-body scattering amplitude, we pick up four factors of $\sqrt{i}$ from the external legs, so that the net scattering amplitude involves an awkward factor of "i". If we now proceed using the generating function approach, we set $n = 2$ and then write

$$i^{n-1}V(\zeta\frac{\delta}{\delta\alpha},\frac{\delta}{\delta\bar\alpha}) = i\frac{1}{2}\int d^3xd^3x'V(x-x')\frac{\delta}{\delta\alpha(x)}\frac{\delta}{\delta\alpha(x')}\frac{\delta}{\delta\bar\alpha(x')}\frac{\delta}{\delta\bar\alpha(x)} \qquad (8.52)$$

Notice how the amplitude for scattering two particles is now $iV(x-x')$ (or $iV(x-x')/\hbar$ if we reinstate Planck's constant). We can now formally denote the scattering vertex as

$$\tfrac{\delta}{\delta\alpha(2)}\quad \tfrac{\delta}{\delta\alpha(1)}$$
$$\tfrac{1}{2}$$
$$\tfrac{\delta}{\delta\bar\alpha(2)}\quad \tfrac{\delta}{\delta\bar\alpha(1)} \qquad (8.53)$$

This gives rise to the following expression for the generating functional

$$\mathcal{S}_I[\bar\alpha,\alpha] = \exp\Big[\frac{1}{2}\ \tfrac{\delta}{\delta\alpha(2)}\ \ \tfrac{\delta}{\delta\alpha(1)}\ \ \tfrac{\delta}{\delta\bar\alpha(2)}\ \ \tfrac{\delta}{\delta\bar\alpha(1)}\ \Big]\exp\Big[\bar\alpha \longleftarrow \alpha\Big]$$

for the S-matrix of interacting particles.

As in the one-particle scattering case, the differential operators acting on the bare S-matrix, glue the scattering vertices to the ends of the propagators, and thereby generate a sum of all possible Feynman diagrams. Once again, we are supposed to formally expand the exponentials on both sides, e.g.

$$\mathcal{S}_I[\bar\alpha,\alpha] = \sum_{n,m}\frac{1}{n!m!}\Big[\frac{1}{2}\ \tfrac{\delta}{\delta\alpha(2)}\ \ \tfrac{\delta}{\delta\alpha(1)}\ \ \tfrac{\delta}{\delta\bar\alpha(2)}\ \ \tfrac{\delta}{\delta\bar\alpha(1)}\Big]^n\Big[\bar\alpha \longleftarrow \alpha\Big]^m \qquad (8.54)$$

Let us again look at some of the leading diagrams that appear in this process. For instance

$$\frac{1}{2!}\Big[\frac{1}{2}\ \tfrac{\delta}{\delta\alpha(2)}\ \ \tfrac{\delta}{\delta\alpha(1)}\ \ \tfrac{\delta}{\delta\bar\alpha(2)}\ \ \tfrac{\delta}{\delta\bar\alpha(1)}\Big]\Big[\bar\alpha \longleftarrow \alpha\Big]^2 = \frac{1}{2}\Big[\ \ +\ \ \Big].$$

We shall see later that these are the Hartree and Fock contributions to the Ground-state energy. The prefactor of $\frac{1}{2}$ arises here because there are two distinct ways of contracting the vertices with the propagators. At each of the vertices in these diagrams, we must integrate over the space-time coordinates and sum over the spins. Since spin is conserved along each propagator, so this means that each loop has a factor of $(2S+1)$ associated with the spin sum. Once again, for fermions, we have to be careful about the minus signs. For each particle loop, there is always an odd number of fermion propagators propagating backwards in time, and this gives rise to a factor

$$\zeta(2S+1) = -(2S+1) \qquad (8.55)$$

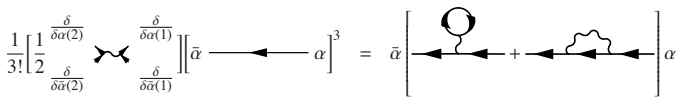
per fermion loop. The algebraic rendition of these Feynman diagrams is then

$$\frac{1}{2}\int d1d2V(1-2)\Big[(2S+1)^2G(0,0^-)^2+\zeta(2S+1)G(1-2)G(2-1)\Big] \tag{8.56}$$

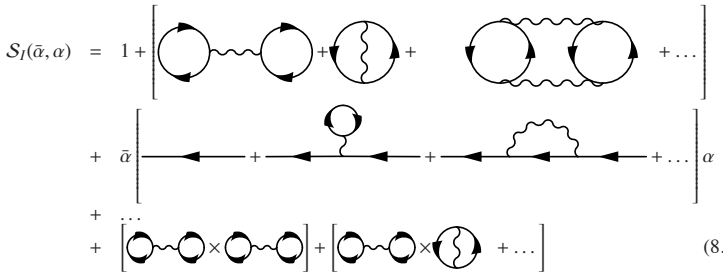
Notice finally, that the first Hartree diagram contains a propagator which "bites its own tail". This comes from a contraction of the density operator,

$$-i\sum_\sigma \langle \ldots \psi_\sigma{}^\dagger(\mathbf{x},t)\psi_\sigma(\mathbf{x},t)\ldots\rangle = \zeta(2S+1)G(\mathbf{x},0^-) \tag{8.57}$$

and since the creation operator lies to the left of the destruction operator, we pick up a minus sign for fermions. As a second example, consider



corresponding to the Hartree and Fock corrections to the propagator. Notice how a similar minus sign is associated with the single fermion loop in the Hartree self-energy. By convention the numerical prefactors are implicitly absorbed into the Feynman diagrams, by introducing two more rules: one which states that each fermion loop gives a factor of ζ, the other which relates the numerical pre-factor to the symmetry of the Feynman diagram. When we add all of these terms, the S-matrix becomes



(8.58)

The diagrams on the first line are "linked-cluster" diagrams: they describe the creation of virtual particle-hole pairs in the vacuum. The second-line of diagrams are the one-leg diagrams, which describe the one-particle propagators. There are also higher order diagrams (not shown) with $2n$ legs, coupled to the source terms, corresponding to the n-particle Green's functions. The diagrams on the third line are "unlinked" diagrams. We shall shortly see that we can remove these diagrams by taking the logarithm of the S-matrix.

8.2.1 Symmetry factors

Remarkably, in making the contractions of the S-matrix, the prefactors in terms like eq. (8.54) are almost completely absorbed by the combinatorics. Let us examine the number of ways of making the contractions between the two terms in (8.54). Our procedure for constructing a diagram is illustrated in Fig. 8.1

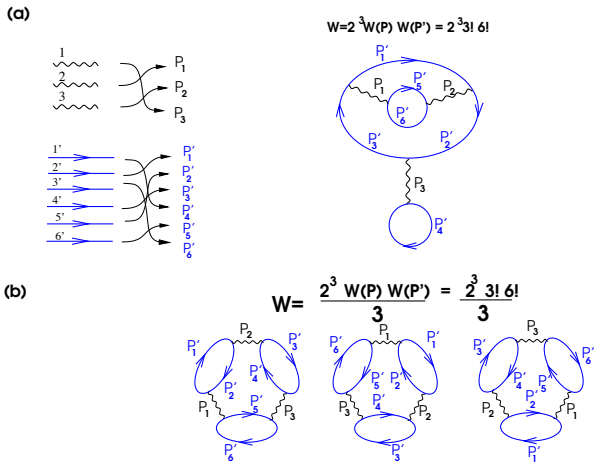


Figure 8.1: (a) Showing how six propagators and three interaction lines can be arranged on a Feynman diagram of low symmetry ($p = 1$). (b) In a Feynman diagram of high symmetry, each possible assignment of propagators and interaction lines to the diagram belongs to a $p-$ tuplet of topologically equivalent assignments, where p is the order of the symmetry group of permutations under which the topology of the diagram is unchanged. In the example shown above, $p = 3$ is the order of the symmetry group. In this case, we need to divide the number of assignments W by a factor of p.

1. We label each propagator on the Feynman diagram 1 through m and label each vertex on the Feynman diagram (1) through (n).

2. The process of making a contraction corresponds to identifying each vertex and each propagator in (8.54) with each vertex and propagator in the Feynman diagram underconstruction. Thus the P'_r th propagator is placed at position r on the Feynman diagram, and the P_k-th interaction line is placed at position k on the Feynman diagram, where P is a permutation of $(1,\ldots n)$ and P' a permutation of $(1,\ldots,m)$.

3. Since each interaction line can be arranged 2 ways at each location, there are $2^n W(P) = 2^n n!$ ways of putting down the the interaction vertices and $W(P') = m!$ ways of putting down the propagators on the Feynman diagram, giving a total of $W = 2^n n!m!$ ways.

4. The most subtle point is notice that if the topology of the Feynman graph is invariant under certain permutations of the vertices, then the above procedure overcounts the number of independent contractions by a "symmetry factor" p, where p is the dimension of the set of permutations under which the topology of the diagram is unchanged. The point is, that each of the $2^n n!m!$ choices made in (2) actually belongs to a $p-$ tuplet of different choices which have actually paired up the propagators and vertices in exactly the same configuration. To adjust for this overcounting, we need to divide the number of choices by the symmetry factor p, so that the number of ways of making the same Feynman graph is

$$W = \frac{2^n n!m!}{p} \tag{8.59}$$

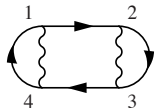
As an example, consider the simplest diagram,

(8.60)

This diagram is topologically invariant under the group of permutations

$$\mathcal{G} = \{(12),(21)\} \tag{8.61}$$

so $p = 2$. In a second example

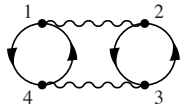


(8.62)

the invariance group is

$$\mathcal{G} = \{(1234),(3412)\} \tag{8.63}$$

so once again, $p = 2$. By contrast, for the diagram



(8.64)

the invariance group is

$$\mathcal{G} = \{(1234),(3412),(2143),(4321)\} \tag{8.65}$$

so that $p = 4$.

8.2.2 Linked Cluster Theorem

One of the major simplifications in developing a Feynman diagram expansion arise because of the Linked Cluster Theorem. Ultimately, we are more interested in calculating the logarithm of the S-matrix, $\ln S(\bar{\eta},\eta)$. This quantity determines both the energy shift due to interactions, but also, it provides the n-particle (connected) Green's functions. In the Feynman diagram expansion of the S-matrix, we saw that there are two types of diagram: linked-cluster diagrams, and unlinked diagrams, which are actually products of linked-cluster diagrams. The linked cluster theorem states that the logarithm of the S-matrix involves just the sum of the linked cluster diagrams:

$$\ln S_I[\bar{\eta},\eta] = \sum \{\text{Linked Cluster Diagrams}\} \tag{8.66}$$

To show this result, we shall employ a trick called the "replica trick", which takes advantage of the relation

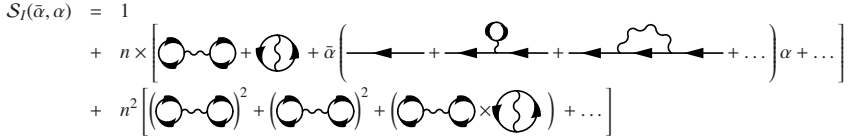
$$\ln S = \lim_{n\to 0}\left[\frac{S^n - 1}{n}\right] \tag{8.67}$$

In other words, if we expand S^n as a power-series in n, then the linear coefficient in the expansion will give us the logarithm of S. It proves much easier to evaluate S^n diagramatically. To do this, we introduce n identical, but independent replicas of the original system, each "replica" labelled by $\lambda = (1,n)$. The Hamiltonian of the replicated system is just $H = \sum_{\lambda=1,n}$ and since the operators of each replica live in a completely independent Hilbert space, they commute. This permits us to write

$$(S_I[\bar{\eta},\eta])^n = \langle\phi|T\exp\left[-i\int_{-\infty}^{\infty} dt \sum_{\lambda=1,n}\left(V(\psi_\lambda{}^\dagger,\psi_\lambda) + \text{source terms}\right)\right]|\phi\rangle \tag{8.68}$$

When we expand this, we will generate exactly the same Feynman diagrams as in S, excepting that now, for each linked Feynman diagram, we will have to multiply the amplitude by N. The diagram expansion for interacting fermions will look like

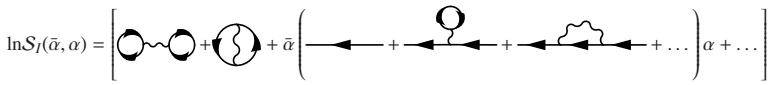
$\mathcal{S}_I(\bar{\alpha},\alpha) =$



(8.69)

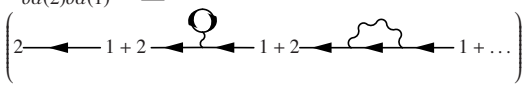
from which we see that the coefficient of N in the replica expansion of S^N is equal to the sum of the linked cluster diagrams, so that

$\ln\mathcal{S}_I(\bar{\alpha},\alpha) =$



By differentiating the log of the S-matrix with respect to the source terms, extract the one-particle Green's functions as the sum of all two-leg diagrams

$$G(2-1) = \zeta\frac{\delta^2 \ln \mathcal{S}_I(\bar\alpha,\alpha)}{\delta\bar\alpha(2)\delta\alpha(1)} = \sum\{\text{Two leg diagrams}\}$$



(8.70)

This is a quite non-trivial result. Were we to have attempted a head-on Feynman diagram expansion of the Green's function using the Gell Mann Lowe theorem,

$$G(1-2) = -i\frac{\langle\phi|T\,S\,\psi(1)\psi^\dagger(2)|\phi\rangle}{\langle\phi|S\,|\phi\rangle} \tag{8.71}$$

we would have to consider the quotient of two sets of Feynman diagrams, coming from the contractions of the denominator and numerator. Remarkably, the unlinked diagrams of the S matrix in the numerator cancel the unlinked diagrams appearing in the Wick expansion of the denominator, leaving us with this elegant expansion in terms of two-leg diagrams.

The higher order derivatives w.r.t. α and $\bar\alpha$ correspond to the connected n-body Green's functions

Example 8.1: By introducing a chemical potential source term into the original Hamiltonian,

$$H = \int d^3x\delta\phi(x,t)\hat\rho(x) \tag{8.72}$$

show that the change in the logarithm of the S-matrix is

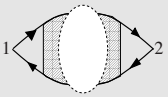
$$\ln S\,[\phi] = \ln S\,[0] + \frac{1}{2}\left[\delta\phi(1)\quad\quad\delta\phi(2)\right] \tag{8.73}$$

where

(8.74)

denotes the sum of all diagrams that connect two "density" vertices. Use this result to show that the time-ordered density correlation function is given by

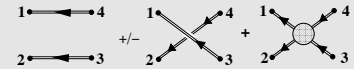
$$-i\langle\phi|T\delta\rho(1)\delta\rho(2)|\phi\rangle = i\frac{\delta^2}{\delta\phi(1)\delta\phi(2)}\ln S\,[\phi] = i$$



(8.75)

Example 8.2: Expand the S-matrix to quadratic order in α and $\bar\alpha$, and use this to show that the two-particle Green's function is given by

$$\frac{1}{S\,[\bar\alpha,\alpha]}\frac{\delta^4 S}{\delta\bar\alpha(1)\delta\bar\alpha(2)\delta\alpha(3)\delta\alpha(4)} = -\langle\phi|T[\psi(1)\psi(2)\psi^\dagger(3)\psi^\dagger(4)]|\phi\rangle$$



(8.76)

Show that the last term, which is the connected two-particle Green's function, is the quartic term coefficient in the expansion of $\ln S\,[\bar\alpha,\alpha]$.

8.3 Feynman rules in momentum space

Though it is easiest to motivate the Feynman rules in real space, practical computations are much more readily effected in momentum space. We can easily transform to momentum space by expanding each interaction line and Green's function in terms of their Fourier components:

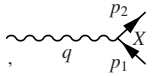
$$1 \longrightarrow 2 = G(X_1 - X_2) = \int \frac{d^dp}{(2\pi)^d}G(p)e^{ip(X_1-X_2)}$$

$$1 \sim\sim 2 = V(X_1 - X_2) = \int \frac{d^dq}{(2\pi)^d}V(q)e^{iq(X_1-X_2)} \tag{8.77}$$

where we have used a short-hand notation $p = (\mathbf{p},\omega), q = (\mathbf{q},\nu), X = (\mathbf{x},t)$, and $pX = \mathbf{p}\cdot\mathbf{x} - \omega t$. We can deal with source terms in similar way, writing

$$\alpha(X) = \int \frac{d^dp}{(2\pi)^d}e^{ipX}\alpha(p). \tag{8.78}$$

Having made these transformations, we see that the space-time co-ordinates associated with each vertex, now only appear in the phase factors. At each vertex, we can now carry out the integral over all space-time co-ordinates, which then imposes the conservation of frequency and momentum at each vertex.



$$= \int d^dX e^{i(p_1-p_2-q)X} = (2\pi)^d\delta^{(d)}(p_1 - p_2 - q) \tag{8.79}$$

Since momentum and energy are conserved at each vertex, this means that there is one independent energy and momentum per loop in the Feynman diagram. Thus the transformation from real-space, to momentum space Feynman rules is effected by replacing the sum over all space-time co-ordinates by the integral over all loop momenta and frequency. (Table 8.2). The convergence factor

$$e^{i\omega O^+} \tag{8.80}$$

is included in the loop integral. This term is only really needed when the loop contains a single propagator, propagating back to the point from which it eminated. In this case, the convergence factor builds in the information that the corresponding contraction of field operators is normal ordered.

Actually, since all propagators and interaction variables depend only on the difference of position, the integral over all n space-time co-ordinates can be split up into an integral over the center-or-mass co-ordinate

$$X_{cm} = \frac{X_1 + X_2 + \ldots X_n}{n} \tag{8.81}$$

and the relative co-ordinates

$$\tilde{X}_r = X_r - X_1, \qquad (r > 1), \tag{8.82}$$

as follows

$$\prod_{r=1,n} d^d X_r = d^d X_{cm} \prod_{r=2,n} d^d \tilde{X}_r \tag{8.83}$$

The integral over the $\tilde{X}_r$ imposes momentum and frequency conservation, whilst the integral over X_{cm} can be factored out of the diagram, to give an overall factor of

$$\int d^d X_{cm} = (2\pi)^d \delta^{(d)}(0) \equiv VT \tag{8.84}$$

where V is the volume of the system, and T the time over which the interaction is turned on. This means that the proper expression for the logarithm of the S-matrix is

$$\ln(S) = VT \sum \{ \text{ linked cluster diagrams in momentum space}\}. \tag{8.85}$$

In other words, the phase-factor associated with the S-matrix grows extensively with the volume and the time over which the interactions act.

8.3.1 Relationship between energy, and the S-matrix

One of the most useful relationships of perturbation theory, is the link between the S-matrix and the ground-state energy, originally derived by Jeffrey Goldstone[3]. Here the basic idea is very simple. When we turn on the interaction, the ground-state energy changes which causes the phase of the S-matrix to evolve. If we turn on the interaction for a time T, then we expect that for sufficiently long times, the phase of the S-matrix will be given by $-i\Delta ET$:

$$S[T] = \langle -\infty | \hat{U}(T/2) U^\dagger(-T/2) | \infty \rangle \propto e^{-i\Delta ET} \tag{8.86}$$

where $\Delta E = E_g = E_o$ is the shift in the ground-state energy as a result of interactions. This means that at long times,

$$\ln(S[T]) = -i\Delta ET + \text{constant} \tag{8.87}$$

But from the linked cluster theorem, we know that

$$\mathrm{S} = VT \sum \{\text{linked clusters in momentum space}\} \tag{8.88}$$

which then means that the change in the ground-state energy due to interactions is given by

$$\boxed{\Delta E = iV \sum \{\text{linked clusters in momentum space}\}} \tag{8.89}$$

To show this result, let us turn on the interaction for a period of time T, writing the ground-state S-matrix as

$$S[T] = \langle -\infty | \hat{U}(T/2) U^\dagger(-T/2) | \infty \rangle \tag{8.90}$$

If we insert a complete set of energy eigenstates $\underline{1} = \sum_\lambda |\lambda\rangle\langle\lambda|$ into this expression for the S-matrix, we obtain

$$S[T] = \sum_\lambda \langle -\infty | \hat{U}(T/2) | \lambda \rangle \langle \lambda | U^\dagger(-T/2) | \infty \rangle \tag{8.91}$$

In the limit $T \to \infty$, the only state with an overlap with the time-evolved state $U^\dagger(-T/2)|\phi_o\rangle$ will be the true ground-state $|\psi_g\rangle$ of the interacting system, so we can write

$$S(T) \to \mathcal{U}(T/2)\mathcal{U}^\dagger(-T/2) \tag{8.92}$$

where $\mathcal{U}(\tau) = \langle -\infty | \hat{U}(\tau/2) | \phi \rangle$. Now differentiating the first term in this product, we obtain

$$\begin{aligned} \frac{\partial}{\partial \tau}\mathcal{U}(\tau) &= \frac{\partial}{\partial \tau}\langle \psi_o | e^{iH_o\tau/2} e^{-iH\tau/2} | \psi_g \rangle \\ &= \frac{i}{2}\langle \psi_o | \{H_o U(\tau/2) - U(\tau/2) H\} | \psi_g \rangle \\ &= -\frac{i\Delta E}{2}\mathcal{U}(\tau) \end{aligned} \tag{8.93}$$

Similarly, $\frac{\partial}{\partial \tau}\mathcal{U}^\dagger(-\tau) = -\frac{i\Delta E}{2}\mathcal{U}^\dagger(-\tau)$, so that

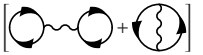
$$\frac{\partial S(T)}{\partial T} = -i\Delta E S(T) \tag{8.94}$$

which proves the original claim.

8.4 Examples

8.4.1 Hartree Fock Energy

As a first example of the application of Feynman diagrams, we use the linked cluster theorem to expand the ground-state energy of an interacting electron gas to first order. To leading order in the interaction strength, the shift in the ground-state energy is given by

$E_g = E_o + iV \Big[$  $\Big]$ (8.95)

corresponding to the Hartree, and Fock contributions to the ground-state energy. Writing out this expression explicitly, noting that the symmetry factor associated with each diagram is $p = 2$, we obtain

$$\Delta E_{HF} = \frac{iV}{2}\int \frac{d^3kd^3k'}{(2\pi)^6}\frac{d\omega d\omega'}{(2\pi)^2}e^{i(\omega+\omega')\delta}\Big[(-[2S+1])^2(iV_{\mathbf{q}=\mathbf{0}}) + (-[2S+1])(iV_{\mathbf{k}-\mathbf{k}'})\Big]G(k)G(k')$$

In the last chapter (6.74), we obtained the result

$$\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle = -i\int\frac{d\omega}{2\pi}G(\mathbf{k},\omega)e^{i\omega\delta} = f_{\mathbf{k}} = \theta(\mathbf{k}_F - |\mathbf{k}|) \tag{8.96}$$

so that the shift in the ground-state energy is given by

$$\Delta E_{HF} = \frac{V}{2}\int\frac{d^3kd^3k'}{(2\pi)^6}\Big[(2S+1)^2(V_{\mathbf{q}=\mathbf{0}}) - (2S+1)(V_{\mathbf{k}-\mathbf{k}'})\Big]f_{\mathbf{k}}f_{\mathbf{k}'} \tag{8.97}$$

In the first term, we can identify $\rho = (2S+1)\sum f_{\mathbf{k}}$ as the density, so this term corresponds to the classical interaction energy of the Fermi gas. The second term is the exchange energy. This term is present because the spatial wavefunction of parallel spin electrons is antisymmetric, which keeps them apart, producing a kind of "correlation hole" between parallel spin electrons.

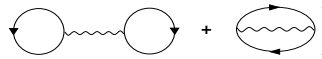
Let us examine the exchange correlation term in more detail. To this end, it is useful to consider the equal time density correlation function,

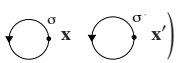
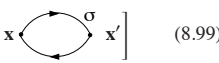
$$C_{\sigma\sigma'}(\vec{x}-\vec{x'}) = \langle\phi_0| : \rho_\sigma(x)\rho_{\sigma'}(x') : |\phi_0\rangle$$

In real space, the Hartree Fock energy is given by

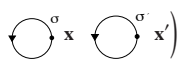
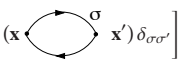
$$\begin{aligned}\langle\phi_0|\hat{V}|\phi_0\rangle &= \frac{1}{2}\sum_{\sigma,\sigma'}\int d^3xd^3yV(\vec{x}-\vec{y})\langle\phi_0| : \hat{\rho}_\sigma(\vec{x})\rho_{\sigma'}(\vec{y}) : |\phi_0\rangle \\ &= \frac{1}{2}\sum_{\sigma,\sigma'}\int d^3xd^3yV(\vec{x}-\vec{y})C_{\sigma\sigma'}(\vec{x}-\vec{y})\end{aligned} \tag{8.98}$$

Now if we look at the real-space Feynman diagrams for this energy,

$\Delta E = i\Big[$  $\Big]$

$= -\frac{1}{2}\sum_{\sigma\sigma'}\int_{\mathbf{x},\mathbf{x}'}V(\mathbf{x}-\mathbf{x}')\Big[\Big($  $+$ $\Big) +$  $\Big]$ (8.99)

since each interaction line contributes a $iV(\mathbf{x}-\mathbf{x}')$ to the total energy, we deduce that the Feynman diagram for the equal time density correlation functions are

$C_{\sigma\sigma'}(\mathbf{x}-\mathbf{y}) = -\Big[\Big($  $+$ $\Big) + ($  $)\delta_{\sigma\sigma'}\Big]$ (8.100)

Written out explicitly,

$$\begin{aligned}C_{\sigma\sigma'}(\vec{x}-\vec{y}) &= -\Big[\overbrace{(-G(\vec{0},0^-))^2}^{-i\rho_0}) - \delta_{\sigma\sigma'}G(\vec{x}-\vec{y},0^-)G(\vec{y}-\vec{x},0^-)\Big] \\ &= \rho_0^2 + \delta_{\sigma\sigma'}G(\vec{x}-\vec{y},0^-)G(\vec{y}-\vec{x},0^-)\end{aligned} \tag{8.101}$$

where we have identified $G(\vec{0},0^-) = i\rho_0$ with the density of electrons per spin. From this we see that $C_{\uparrow\downarrow}(\vec{x}-\vec{y}) = \rho_0^2$ is independent of separation- there are no correlations between the up and down-spin density in the non-interacting electron ground state. However, the correlation function between parallel spin electrons contains an additional term. We can calculate this term from the equal time electron propagator, which in real space is given by

$$\begin{aligned}G(\vec{x},0^-) &= \int_{\mathbf{k}}G(\mathbf{k},0^-)e^{i\mathbf{k}\cdot\mathbf{x}} = i\int_{\mathbf{k},\ \frac{\sin kr}{kr}}f_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}} \\ &= i\int_{k<k_F}\frac{k^2dk}{2\pi^2}\overbrace{\int\frac{d\cos\theta}{2}e^{ikr\cos\theta}} \\ &= \frac{i}{2\pi^2r^3}[\sin(k_Fr) - k_Fr\cos(k_Fr)] = i\rho_0P(k_Fx)\end{aligned} \tag{8.102}$$

where $\rho_0 = \frac{k_F^3}{6\pi^2}$ is the density, while

$$P(x) = 3\left(\frac{\sin x - x\cos x}{x^3}\right) = \frac{3}{x}j_1(x) \tag{8.103}$$

and $j_1(x)$ is the $l = 1$ spherical Bessel function. The density correlation function of parallel spin fermions then takes the form

$$C_{\uparrow\uparrow}(r) = \rho_0^2\left(1 - [P(k_Fr)]^2\right)$$

This function is shown in Fig. 8.2: at $r = 0$ it goes to zero, corresponding to the fact that the probability to find two "up" electrons in the same place actually vanishes. It is this hole in the correlation function that gives the interacting electron fluid a pre-disposition towards the development of ferromagnetism and triplet paired superfluids.

Before we end this section, let us examine the Hartree Fock energy for the Coulomb gas. Formally, with the Coulomb interaction the Hartree interaction becomes infinite, but in practice, we need not worry, because to stabilize the charged Fermi gas, we need to compensate the charge of the Fermi gas with a uniformly charged background. Provided the Fermi gas is uniform, the classical Coulomb energy of the combined system is then identically zero. The leading order expression for the ground-state energy of the compensated Coulomb gas of Fermions is then

$$\frac{E_g}{V} = (2S+1)\int_{\mathbf{k}}\frac{\hbar^2k^2}{2m}f_{\mathbf{k}} - \frac{(2S+1)}{2}\int_{\mathbf{k},\mathbf{k}'}f_{\mathbf{k}}f_{\mathbf{k}'}\frac{e^2}{\epsilon_0(\mathbf{k}-\mathbf{k})^2} \tag{8.104}$$

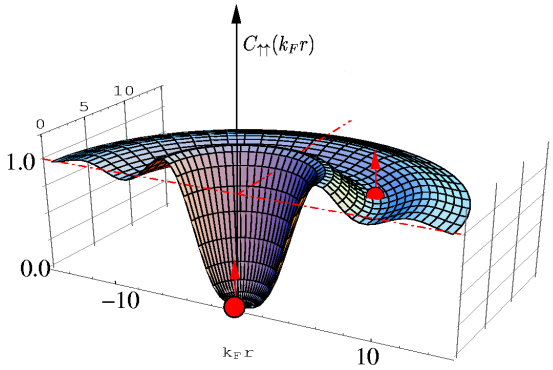


Figure 8.2: "Correlation hole". The equal time correlation function $C_{\uparrow\uparrow}(k_F r)$ for the non-interacting Fermi gas. Notice how this function vanishes at the origin, corresponding to a vanishing probability to find two "up" electrons at the same location in space.

A careful evaluation of the above integrals (see Problem 8.1) gives

$$\frac{E_g}{V} = \rho\left[\frac{3}{5}\epsilon_F - \frac{3e^2k_F}{4\pi}\right]$$

where $\rho = (2S+1)k_F^3/(3\pi^2)$ is the density of particles. An important parameter for the electron gas is the dimensionless separation of the electrons. The separation of electrons R_e in a Fermi gas is defined by

$$\frac{4\pi R_e^3}{3} = \rho^{-1}$$

where ρ is the density of electrons. The dimensionless separation r_s is defined as $r_s = R_e/a_B$ where $a_B = \frac{\hbar^2 4\pi\epsilon_0}{me^2}$ is the Bohr radius, so that

$$r_s = \frac{1}{\alpha k_F a_B} \tag{8.105}$$

where $\alpha = \left(\frac{4}{9\pi}\right)^{\frac{1}{3}} \approx 0.521$. Using r_s, we can re-write the energy of the electron gas as

$$\frac{E}{\rho V} = \frac{3}{5}\frac{R_Y}{\alpha^2 r_s^2} - \frac{3}{2\pi}\frac{R_Y}{\alpha r_s}$$

$$= \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_S}\right)R_Y \tag{8.106}$$

where $R_Y = \frac{\hbar^2}{2ma_B^2} = 13.6eV$ is the Rydberg energy. From this, we see that the most strongly correlated limit of the electron gas is the *dilute limit*.

8.4.2 Electron in a scattering potential

As an illustration of the utility of the Feynman diagram approach, we now consider an electron scattering off an attractive central scattering potential. Here, by resumming the Feynman diagrams, it is easy to show how in dimensions $d \leq 2$, an arbitrarily weak attractive potential gives rise to bound-states.

The Hamiltonian is given by

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + H_{sc} \tag{8.107}$$

where $\epsilon_{\mathbf{k}} = k^2/2m - \mu$ and the scattering potential is given by

$$H_{sc} = \int d^3x \psi^\dagger(x)\psi(x)U(x) \tag{8.108}$$

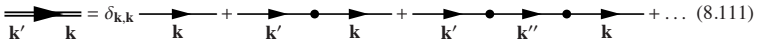
If we Fourier transform the scattering potential, writing

$$U(x) = \int_{\mathbf{q}} U(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{x}} \tag{8.109}$$

then the scattering potential becomes

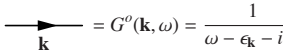
$$H_{sc} = \int_{\mathbf{k},\mathbf{k}'} \underbrace{U_{\mathbf{k}-\mathbf{k}'}}_{\text{amplitude to transfer momentum } \mathbf{k}-\mathbf{k}'} c^\dagger_{\mathbf{k}} c_{\mathbf{k}'} \tag{8.110}$$

The Feynman diagrams for the one-electron Green's function are then



(8.111)

where



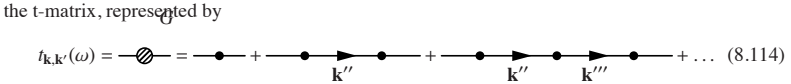
(8.112)

denotes the propagator in the absence of potential scattering and

(8.113)

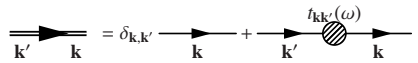
is the basic scattering vertex. The first diagram represents the amplitude to be transmitted without scattering; subsequent diagrams represent multiple scattering processes involving one, two three

and more scattering events. We shall lump all scattering processes into a single amplitude, called the t-matrix, represented by



$$t_{\mathbf{k},\mathbf{k}'}(\omega) = \quad = \quad + \quad + \quad + \ldots \tag{8.114}$$

With this short-hand notation, the diagrams for the electron propagator become

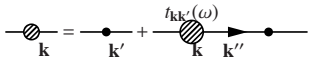


(8.115)

Written out as an equation, this is

$$G(\mathbf{k},\mathbf{k}',\omega) = \delta_{\mathbf{k},\mathbf{k}'}G^o(\mathbf{k},\omega) + G^o(\mathbf{k},\omega)t_{\mathbf{k},\mathbf{k}'}(\omega)G^o(\mathbf{k}',\omega) \tag{8.116}$$

If we look at the second, third and higher scattering terms in the t-matrix, we see that they are a combination of the t-matrix plus the bare scattering amplitude. This enables us to re-write the t-matrix as the following self-consistent set of Feynman diagrams



(8.117)

Written out explicitly, this is

$$t_{\mathbf{k}\mathbf{k}'}(\omega) = U_{\mathbf{k}-\mathbf{k}'} + \sum_{\mathbf{k}''} U_{\mathbf{k}-\mathbf{k}''}G^o(\mathbf{k}'',\omega)t_{\mathbf{k}''\mathbf{k}'}(\omega) \tag{8.118}$$

Equations (8.116) and (8.118) fully describe the scattering off the impurity.

As a simplified example of the application of these equations, let us look at the case of s-wave scattering off a point-like scattering center:

$$U(\mathbf{x}) = U\delta^{(d)}(\mathbf{x}) \tag{8.119}$$

In this case, $U(\mathbf{q}) = U$ is independent of momentum transfer. By observation, this means that the t-matrix will also be independent of momentum, i.e. $t_{\mathbf{k},\mathbf{k}'}(\omega) = t(\omega)$. The equation for the t-matrix then becomes

$$t(\omega) = U + U\sum_{\mathbf{k}''} G^o(\mathbf{k}'',\omega)t(\omega) \tag{8.120}$$

or

$$t(\omega) = \frac{U}{1 - UF(\omega)} \tag{8.121}$$

where

$$\begin{aligned} F(\omega) &= \int \frac{d^dp}{(2\pi)^d}\frac{1}{\omega - \epsilon_{\mathbf{k}} + i\delta_{\mathbf{k}}} \\ &= \int_0^{\Lambda} d\epsilon N(\epsilon)\frac{1}{\omega - \epsilon + i\delta\mathrm{sign}(\epsilon)} \end{aligned} \tag{8.122}$$

and $N(\epsilon)$ is the density of states. A high-energy cut-off has been introduced to guarantee the convergence of the integral. Physically, such a cut-off corresponds to the energy scale, beyond which ,the scattering potential no longer behaves as a point potential. At low energies, $F(\omega) < 0$, so that if $U < 0$, there is the possibility of poles in the t-matrix, corresponding to bound-states.

As we have derived it, our scattering t-matrix describes scattering in the presence of a Fermi sea. To recover free particle behavior, we imagine that the Fermi sea is empty, so that the chemical potential is zero so that

$$\epsilon_{\mathbf{k}} = \frac{k^2}{2m} \tag{8.123}$$

In d-dimensions, the density of states is given by

$$N(\epsilon) \propto k^{d-1}\frac{dk}{d\epsilon} \propto \epsilon^{\frac{d}{2}-1} \tag{8.124}$$

The low energy behavior of $F(\omega)$ is then given by

$$F(\omega) \propto -\omega^{d/2-1} \tag{8.125}$$

This quantity diverges in dimensions $d \leq 2$, so that there will be bound-states for arbitrarily small attractive potentials $U < 0$. In two dimensions, the density of states is $N(\omega) = N(0)$and $F(\omega) = -N(0)\ln\frac{\Lambda}{-\omega}$, so that for attractive $U = -|U|$,

$$t(\omega) = -\frac{|U|}{1 - |U|N(0)\ln\frac{\Lambda}{-\omega}} = \frac{1}{N(0)\ln\left(\frac{\omega_o}{-\omega}\right)} \tag{8.126}$$

where $\omega_o = \Lambda e^{-\frac{1}{|U|N(0)}}$, giving rise to a bound-state at energies $\omega = -\omega_o$.

Remarks

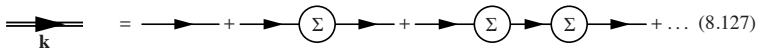
- The energy scale ω_o can not be written as a power-series in U, and as such, is an elementary example of a "non-perturbative" result. The bound-state appears because an infinite class of Feynman diagrams have been resummed.
- The appearance of a bound-state for electrons scattering off an arbitrarily weak attractive potential is similar to the Cooper instability.

8.5 The self-energy

The concept of the self-energy enables us to understand the feedback of the interacting environment on a propagating particle. This is one of the most important examples of the power of Feynman diagram resummation.

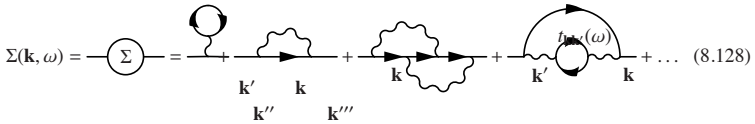
Let us consider the Greens function of a fermion in an interacting environment. Every diagram contributing to the propagator consists of a sequence of free propagators separated by various many-body scattering processes. The self-energy sums the amplitude for all of these intermediate

scattering processes into a single entity represented by the symbol Σ. With this conceptual simplification, the propagator has the structure



(8.127)

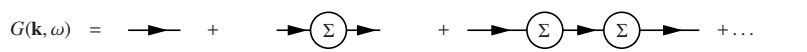
where



(8.128)

denotes the self-energy: the sum of all scattering processes that can not be separated into two by cutting a single propagator. By convention each of these diagrams contain two small stubs (without arrows) that denote the points where the diagram connects with incoming and outgoing propagators. We do not associate any propagator with these stubs. In a rather macabre terminology, the external legs of the self-energy are sometimes said to have been "amputated".

The one-particle propagator can then be expanded as a geometric series involving the self-energy, as follows



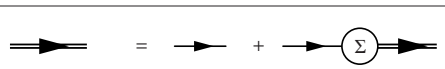
$$= G^0 + G^0\Sigma G^0 + G^0(\Sigma G^0)^2 + \ldots$$
$$= \frac{G_0}{1-\Sigma G^0} = \frac{1}{(G^0(\mathbf{k},\omega))^{-1} - \Sigma(\mathbf{k},\omega)} \tag{8.129}$$

So that

$$G(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k},\omega)} \tag{8.130}$$

Feynman propagator

This heuristic derivation involves the summation of a geometric series, which in general will be outside its radius of convergence, but we may argue the result is true by analytic continuation. Another way to derive the same result is to notice that the second and subsequent terms in the series (8.129) can be re-written in terms of the original Green's function, as follows:



(8.131)

$$G(\mathbf{k},\omega) = G^0(\mathbf{k},\omega) + G^0(\mathbf{k},\omega)\Sigma(\mathbf{k},\omega)G(\mathbf{k},\omega)$$

Dyson equation

This equation is called a "Dyson equation"[2]. Using it to solve for $G(\mathbf{k},\omega)$, we also obtain (8.130). Physically, the self-energy describes the cloud of particle-hole excitations which accompanies the propagating electron, "dressing" it into a quasiparticle. In general, the self-energy has both a real, and an imaginary component.

$$\Sigma(\mathbf{k},\omega - i\delta) = \Sigma'(\mathbf{k},\omega) + i\Gamma(\mathbf{k},\omega). \tag{8.132}$$

The imaginary component to the self-energy describes the rate of decay of the bare fermion, through the emission of particle-hole pairs.

If we use this expression to evaluate the one-particle spectral function, we obtain

$$A(\mathbf{k},\omega) = \frac{1}{\pi}\mathrm{Im}G(\mathbf{k},\omega - i\delta) = \frac{\Gamma(\mathbf{k},\omega)}{[\omega - \epsilon_{\mathbf{k}} - \Sigma'(\mathbf{k},\omega)]^2 + \Gamma(\mathbf{k},\omega)^2} \tag{8.133}$$

If the self-energy is small, we see that this corresponds to a Lorentzian of width Γ centered around a renormalized energy $\epsilon^*_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Sigma'(\mathbf{k},\epsilon^*_{\mathbf{k}})$. If we expand the Lorentzian around this point, we must be careful to write $\omega - \epsilon_{\mathbf{k}} - \Sigma'(\mathbf{k},\omega) = (\omega - \epsilon^*_{\mathbf{k}})Z_{\mathbf{k}}$ where $Z^{-1}_{\mathbf{k}} = (1 - \partial_\omega\Sigma'(\mathbf{k},\omega))|_{\omega=\epsilon^*_{\mathbf{k}}}$. Near the renormalized energy $\omega \sim \epsilon^*_{\mathbf{k}}$,

$$G(\mathbf{k},\omega - i\delta) = \frac{Z_{\mathbf{k}}}{\omega - \epsilon^*_{\mathbf{k}} - i\Gamma^*_{\mathbf{k}}}, \tag{8.134}$$

where, provided $\Gamma^*_{\mathbf{k}}$ is small,

$$\begin{aligned} \epsilon^*_{\mathbf{k}} &= \epsilon_{\mathbf{k}} + \Sigma'(\mathbf{k},\epsilon^*_{\mathbf{k}}), && \text{renormalized energy} \\ \tau^{-1} &= Z_{\mathbf{k}}\Gamma(\mathbf{k},\epsilon^*_{\mathbf{k}}), && \text{Lifetime.} \end{aligned} \tag{8.135}$$

can be interpreted as a "quasiparticle" with energy ϵ^*_{bk} and lifetime $\Gamma^*_{\mathbf{k}}$ (see section 7.8). Now this "quasiparticle peak" is not the only component to the spectral function, because it only contains a weight $Z_{\mathbf{k}}$, while the total weight of the spectral function is unity. The full Green's function is better represented in the form

$$G(\mathbf{k},\omega - i\delta) = \frac{Z_{\mathbf{k}}}{\omega - \epsilon^*_{\mathbf{k}} - i\Gamma^*_{\mathbf{k}}} + G_{\mathrm{inc}}(\mathbf{k},\omega) \tag{8.136}$$

where G_{inc} represents the incoherent particle-hole continuum contribution to the Green's function. This is precisely the form of spectral function expected in a Fermi liquid (7.8), with a sharp quasiparticle pole co-existing with an incoherent background $A_{\mathrm{inc}}(\mathbf{k},\omega)$. From the spectral decomposition (6.117), we can relate $Z_{\mathbf{k}}$ to the overlap between the bare particle and the dressed quasiparticle:

$$Z_{\mathbf{k}} = |\langle \text{q.ptcle } \mathbf{k}\sigma | c^\dagger{}_{\mathbf{k}\sigma}|\phi\rangle|^2 \qquad \text{"Quasiparticle weight".} \tag{8.137}$$

8.5.1 Hartree-Fock Self-energy

The simplest example of the self-energy is the Hartree-Fock self energy, given by the two diagrams

$$\Sigma_{HF}(\mathbf{p},\omega) = \quad + \quad \Sigma$$

$$\Sigma \qquad \Sigma$$

$$= i\int_{\mathbf{p}'}\left\{-(2S+1)V_{\mathbf{q}=0}+V_{\mathbf{p}-\mathbf{p}'}\right\}\int\frac{d\omega}{2\pi}G^0(k)e^{i\omega 0^+} \tag{8.138}$$

Here we see a case where we must include a convergence factor, associated with the normal ordering of the operators inside the interaction. Identifying $\int d\omega G^0(k)e^{i\omega 0^+} = 2\pi i f_{\mathbf{p}'}$, we obtain

$$\Sigma_{HF}(\mathbf{p}) = \int_{|\mathbf{p}'|<k_F}\frac{d^3k'}{(2\pi)^3}\Big[(2S+1)V_{\mathbf{q}=0}-V_{\mathbf{p}-\mathbf{p}'}\Big] \tag{8.139}$$

In the Hartree-Fock approximation, the electron acquires a renormalized energy

$$\epsilon^*_{\mathbf{p}} = \epsilon_{\mathbf{p}} + \Sigma_{HF}(\mathbf{p}) \tag{8.140}$$

but since the Hartree-Fock self-energy is completely static, in this approximation, the quasiparticle has an infinite lifetime. The mass of the quasiparticle is nevertheless renormalized. Suppose we write

$$\frac{\mathbf{p}}{m^*} = \nabla_{\mathbf{p}}\epsilon^*_{\mathbf{p}} = \left[\frac{\mathbf{p}}{m}+\nabla_{\mathbf{p}}\Sigma_{HF}(\mathbf{p})\right] \tag{8.141}$$

then integrating by parts,

$$\nabla_{\mathbf{p}}\Sigma_{HF}(\mathbf{p}) = -\int_{\mathbf{p}'}\nabla_{\mathbf{p}}V_{\mathbf{p}-\mathbf{p}'}f_{\mathbf{p}'} = +\int_{\mathbf{p}'}\nabla_{\mathbf{p}'}V_{\mathbf{p}-\mathbf{p}'}f_{\mathbf{p}'} = -\int_{\mathbf{p}'}V_{\mathbf{p}-\mathbf{p}'}\nabla_{\mathbf{p}'}f_{\mathbf{p}'} \tag{8.142}$$

Writing $\nabla_{\mathbf{p}}f_{\mathbf{p}} = \nabla_{\mathbf{p}}\epsilon^*_{\mathbf{p}}\,(\partial f/\partial\epsilon^*) = -\frac{\mathbf{p}}{m^*}\delta(\epsilon^*_{\mathbf{p}})$, we then obtain

$$\begin{aligned}\nabla_{\mathbf{p}}\Sigma_{HF}(\mathbf{p}) &= \int_{\mathbf{p}'}V_{\mathbf{p}-\mathbf{p}'}\left(\frac{\mathbf{p}'}{m^*}\right)\delta(\epsilon^*_{\mathbf{p}})\\ &= \frac{\mathbf{p}_F}{m^*}\int_{\mathbf{p}'}V_{\mathbf{p}-\mathbf{p}'}(\hat{\mathbf{p}}'\cdot\hat{\mathbf{p}})\delta(\epsilon^*_{\mathbf{p}}) = \left(\frac{\mathbf{p}_F}{m^*}\right)\frac{N(0)}{2}\int\frac{d\Omega_{\mathbf{p}'}}{4\pi}V_{\mathbf{p}-\mathbf{p}'}cos\theta_{\mathbf{p},\mathbf{p}'}\\ &= -\frac{\mathbf{p}}{m^*}F^s_1\end{aligned} \tag{8.143}$$

where $N(0) = m^*p_F/(\pi^2\hbar^3)$ is the renormalized density of states and by analogy with Fermi liquid theory, we have written,

$$F^s_1 = N(0)\int\frac{d\Omega_{\hat{\mathbf{p}}'}}{4\pi}\left(-\frac{V_{\mathbf{p}-\mathbf{p}'}}{2}\right)\cos(\theta_{\mathbf{p},\mathbf{p}'}). \tag{8.144}$$

This is the dipole ($l = 1$) Landau parameter expected in Hartree-Fock theory, where the quasiparticle interaction is given by $f_{\mathbf{p}\sigma,\mathbf{p}\sigma'} = V_{\mathbf{q}=0} - V_{\mathbf{p}-\mathbf{p}'}\delta_{\sigma\sigma'}$, so that $f^s_{\mathbf{p},\mathbf{p}'} = V_{\mathbf{q}=0} - \frac{1}{2}V_{\mathbf{p}-\mathbf{p}'}$ (see eq. (7.36). Combining (8.141) and (8.143), we then obtain

$$\frac{\mathbf{p}}{m^*}(1+F^s_1) = \frac{\mathbf{p}}{m} \tag{8.145}$$

so that the renormalized mass is given by

$$\frac{m^*}{m} = 1 + F^s_1 \tag{8.146}$$

Formally, this result is the same as that derived in Landau Fermi liquid theory (section 7.4.2), using the Hartree-Fock approximation to the quasiparticle interaction (7.36)

$$f^s_{\mathbf{p}\mathbf{p}'} = V_{\mathbf{q}=0} - V_{\mathbf{p}-\mathbf{p}'}. \tag{8.147}$$

However, a more realistic theory would take into account the screening and modification of the interactions by the medium, a subject which we touch on at the end of this chapter.

8.6 Response functions

One of the most valuable applications of Feynman diagrams, is to evaluate response functions. Suppose we couple the interacting system up to an external source field,

$$H(t) = H_o + H_s(t) \tag{8.148}$$

where

$$H_s(t) = -A(t)f(t) \tag{8.149}$$

involves the coupling of an external force to a variable of the system. Examples would include

$$\begin{aligned}H_s(t) &= -\mu_B\int d^3x\vec{\sigma}(x)\cdot\mathbf{B}(x,t), && \text{External magnetic field}\\ H_s(t) &= -\int d^3x\rho(\mathbf{x})\Phi(x,t) && \text{External potential}\end{aligned} \tag{8.150}$$

In each case, the system will respond by a change in the variable $A(t)$. To calculate this change, we use the interaction representation of $H(t)$, so that

$$A_H(t) = U^\dagger(t)A_I(t)U(t) \tag{8.151}$$

where, from chapter 7,

$$U(t) = T\exp\left[-i\int_{-\infty}^{t}H_s(t')dt'\right] \tag{8.152}$$

We shall now drop the subscript I, because $A_I(t) = A(t)$ also corresponds to the Heisenberg representation of H_o. Expanding (8.151) to linear order in H_s, we obtain

$$A_H(t) = A(t) - i\int_{-\infty}^{t}[A(t), H_s(t')]dt' + O(H_s^2) \tag{8.153}$$

Finally, taking expectation values, we obtain

$$\langle A_H(t)\rangle = \langle\phi|A(t)|\phi\rangle - i\int_{-\infty}^{t}\langle\phi|[A(t), H_s(t')]|\phi\rangle dt' \tag{8.154}$$

But if A is zero in the absence of the applied force, i.e. $\langle\phi|A(t)|\phi\rangle = 0$, then the linear response of the system is given by

$$\langle A_H(t)\rangle = \int_{-\infty}^{\infty} dt'\chi(t-t')f(t')dt' \tag{8.155}$$

where

$$\chi(t-t') = i\langle\phi|[A(t), A(t')]|\phi\rangle\theta(t-t') \tag{8.156}$$

is called the "dynamical susceptibility" and $A(t)$ is in the Heisenberg representation of the unperturbed system.

Now in diagramatic perturbation theory, we are able to evaluate time-ordered Green functions, such as

$$\chi^T(1-2) = (-i)^2\langle\phi|TA(1)A(2)|\phi\rangle. \tag{8.157}$$

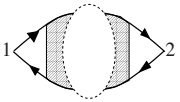
Here, the prefactor $(-i)^2$ has been inserted because almost invariably, A is a bilinear of the quantum field, so that χ^T is a two-particle Greens function. Fortunately, there is a very deep link between the dissipative response function, and the fluctuations associaed with a correlation function, called the "fluctuation-dissipation" theorem. The Fourier transforms of $\mathcal{R}$ and G are both governed by precisely the same many-body excitations, with precisely the same spectral functions, with one small difference: in the complex structure of $\chi(\omega)$, all the poles lie just below the real axis, guaranteeing a retarded response. By contrast, in $\chi^T(\omega)$, the positive and negative energy poles give rise to retarded, and advanced responses, respectively. The spectral decomposition of these functions are then,

$$\begin{aligned}\chi(\omega) &= \sum_\lambda \frac{2|M_\lambda|^2\omega_\lambda}{\omega_\lambda^2 - (\omega+i\delta)^2}\\ \chi^T(\omega) &= i\sum_\lambda \frac{2|M_\lambda|^2\omega_\lambda}{(\omega_\lambda - i\delta)^2 - \omega^2}\end{aligned} \tag{8.158}$$

where $M_\lambda = \langle\lambda|A|\phi\rangle$ is the matrix element between the ground-state and the excited state λ and $\omega_\lambda = E_\lambda - E_g$ is the excitation energy. In this way, the response function can be simply related to the time-ordered response at a small imaginary frequency:

$$\chi(\omega) = -i\chi^T(\omega + i\delta) \tag{8.159}$$

We can obtain the Feynman rules for the time-ordered correlation function, by introducing a source term H_s and calculating the S-matrix $S[f]$. In this case,

$$\frac{\delta^2}{\delta f(1)\delta f(2)}\ln S[f] = -\langle\phi|T[A(1)A(2)]|\phi\rangle = \chi^T(1-2) \equiv$$  (8.160)

Diagramatically, the time-ordered correlation function for the quantity A, is given by

$$\chi^T(\omega) = \sum\{\text{diagrams formed by connecting two "A" vertices together.}\} \tag{8.161}$$

as summarized in Table 8.3.

8.6.1 Magnetic susceptibility of non-interacting electron gas

One of the fundamental qualities of an fermi liquid, is its non-local response to an applied field. Suppose for example, one introduces a localized "delta-function" disturbance in the magnetic field, $\delta B_z(x) = B\delta^3(x)$. Since the fermions have a characteristic wave vector of order k_F, this local disturbance will "heal" over a length-scale of order $l \sim 1/k_F$. Indeed, since the maximum wavevector for low-energy particle-hole excitations is sharply cut-off at $2k_F$, the response produces oscillations in the spin density with a wavelength $\lambda = 2\pi/k_F$ that decay gradually from the site of the disturbance. These oscillations are called "Friedel Oscillations" (Fig. 8.3). In the case of the example just cited, the change in the spin density in response to the shift in the chemical potential is given by

$$\delta M(\vec{x}) = \chi_s(\vec{x})B \tag{8.162}$$

where

$$\chi_s(\vec{x}) = \int_{\mathbf{q}} \chi(\mathbf{q}, \omega = 0)e^{i\vec{q}\cdot\vec{x}} \tag{8.163}$$

is the Fourier transform of the dynamical spin susceptibility. We shall now calculate this quantity as an example of the application of Feynman diagrams.

From the interaction in (8.150) the magnetization is given by

$$\vec{M}(x) = \int d^4x' \underline{\chi}(x - x')\vec{B}(x') \tag{8.164}$$

where

$$\underline{\chi}_{ab}(x) = i\langle\phi|[\sigma^a(x), \sigma^b(0)]|\phi\rangle\theta(t) \tag{8.165}$$

The electron fluid mediates this non-local response. If we Fourier transform this expression, then $\vec{M}(q) = \underline{\chi}(q)\vec{B}(q)$, where (in a relativistic short-hand)

$$\chi_{ab}(q) = i\mu_B^2 \int d^4x \langle\phi|[\sigma^a(x), \sigma^b(0)]|\phi\rangle\theta(t)e^{-iq\cdot x} \tag{8.166}$$

We can relate $\chi_{ab}(\vec{q}, \nu) = -i\chi^T_{ab}(\vec{q}, \nu + i\delta)$ where the time ordered Greens function is given by

$$\begin{aligned}\chi^T_{ab}(q) &= \mu_B^2 \; \sigma^b \; \overset{2\delta^{ab}G(k+q)G(k)}{\overset{k}{\bigcirc}} \; \sigma^a \\ &= -\mu_B^2 \int_{\mathbf{k}} \frac{d\omega}{2\pi} \overbrace{\mathrm{Tr}\left[\sigma^a G(k+q)\sigma^b G(k)\right]}^{2\delta^{ab}G(k+q)G(k)} = \delta_{ab}\chi^T(q).\end{aligned} \tag{8.167}$$

The susceptibility $\chi^T(q)$ is then

$$\chi^T(q) = -2\mu_B^2 \int_{\mathbf{k}} \frac{d\omega}{2\pi}\left[\frac{1}{\omega + \nu - \tilde{\epsilon}_{\mathbf{k}+\mathbf{q}}}\frac{1}{\omega - \tilde{\epsilon}_{\mathbf{k}}}\right] \tag{8.168}$$

where we have invoked the notation $\tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} - i\delta\mathrm{sgn}(\epsilon_{\mathbf{k}})$. The term inside the square brackets has two poles at $\omega = \tilde{\epsilon}_{\mathbf{k}}$ and at $\omega = \tilde{\epsilon}_{\mathbf{k}+\mathbf{q}} - \nu$,

$$\int_\omega = \int \frac{d\omega}{2\pi}\frac{1}{(\tilde{\epsilon}_{\mathbf{k}+\mathbf{q}} - \tilde{\epsilon}_{\mathbf{k}}) - \nu}\left[\frac{1}{\omega + \nu - \epsilon_{\mathbf{k}+\mathbf{q}} + i\delta_{\mathbf{k}+\mathbf{q}}} - \frac{1}{\omega - \epsilon_{\mathbf{k}} + i\delta_{\mathbf{k}}}\right]$$

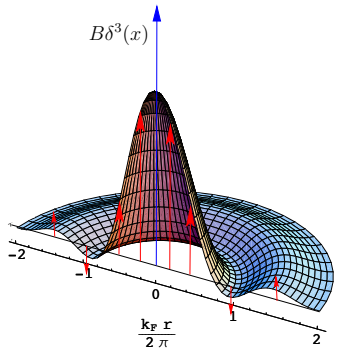


Figure 8.3: "Friedel oscillations in the spin density, in response to a delta-function disturbance in the magnetic field at the origin.These oscillations may be calculated from the Fourier transform of the Lindhard function.

We may carry out the frequency integral by completing the contour in the upper half plane. Each Green function gives a contribution $2\pi i \times$ fermi function, so that

$$\chi^T(q) = -2i\mu_B^2 \int_{\mathbf{k}} \frac{f_{\mathbf{k}+\mathbf{q}} - f_{\mathbf{k}}}{(\tilde{\epsilon}_{\mathbf{k}+\mathbf{q}} - \tilde{\epsilon}_{\mathbf{k}}) - \nu} \tag{8.169}$$

so that the dynamic susceptibility $\chi(\mathbf{q}, \nu) = -i\chi^T(\mathbf{q}, \nu + i\delta)$ is given by

$$\boxed{\chi(\mathbf{q}, \nu + i\delta) = 2\mu_B^2 \int_{\mathbf{k}} \frac{f_{\mathbf{k}+\mathbf{q}} - f_{\mathbf{k}}}{\nu - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) + i\delta} \qquad \text{dynamic spin susceptibility}} \tag{8.170}$$

There are a number of important pieces of physics encoded in the above expression that deserve special discussion:

- Spin Conservation. The total spin of the system is conserved, so that the application of a strictly uniform magnetic field to the fluid can not change the total magnetization. Indeed, in keeping with this expectation, if we take $\vec{q} \to 0$ we find $\lim_{\vec{q}\to 0}\chi(\vec{q}, \nu) = 0$.

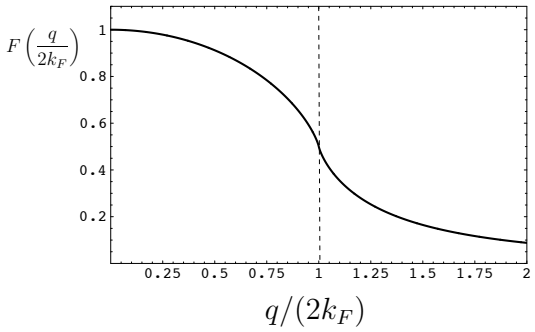


Figure 8.4: "The Lindhard function". The Fourier transform of this function governs the magnetic response of a non-interacting metal to an applied field. Notice the weak singularity around $q/(2k_F) = 1$ that results from the match between the Fermi surface, and the wavevector of the magnetic response.

- Static susceptibility. When we take the limit $\nu \to 0$, we obtain the magnetization response to a spatially varying magnetic field. The static susceptibility is given by

$$\chi(\mathbf{q}) = 2\mu_B^2 \int_{\mathbf{k}} \frac{f_{\mathbf{k}} - f_{\mathbf{k+q}}}{(\epsilon_{\mathbf{k+q}} - \epsilon_{\mathbf{k}})}. \tag{8.171}$$

  This response is finite, because the spins can always redistribute themselves in response to a non-uniform field. When we take the wavelength of the applied field to infinity, i.e $q \to 0$, we recover the Pauli susceptibililty

$$\chi \to 2\mu_B^2 \int_{\mathbf{k}} \left(-\frac{df(\epsilon)}{d\epsilon}\right) = 2\mu_B^2 \int_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}}) = \mu_B^2 N(0), \tag{8.172}$$

  where $N(0) = \frac{mk_F}{\pi^2}$ is the total density of states. The detailed momentum-dependent static susceptibility can be calculated (see below), and is given by

$$\begin{aligned} \chi(\mathbf{q}) &= \mu_B^2 N(0) F(\frac{q}{2k_F}) \\ F(x) &= \frac{1}{4x}(1-x^2)\ln\left|\frac{1+x}{1-x}\right| + \frac{1}{2} \end{aligned} \tag{8.173}$$

  The function $F(x)$ is known as the Lindhard function[4]: it has the property that $F(0) = 1$, while $F'(x)$ has a logarithmic singularity at $|x| = 1$.

- Dissipation and the imaginary part of the susceptibility. The full dynamic spin susceptibility has both a real and an imaginary part, given by

$$\chi(\mathbf{q}, \nu) = \chi'(\mathbf{q}, \nu) + i\chi''(\mathbf{q}, \nu).$$

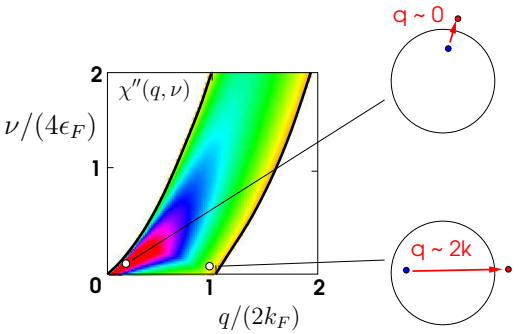


Figure 8.5: Density plot of the imaginary part of the dynamical spin susceptibility, calculated from (8.180) showing the band of width $2k_F$ that spreads up to higher energies. Excitations on the left side of the band correspond to low momentum transfer excitations of electrons from just beneath the Fermi surface to just above the Fermi surface. Excitations on the right hand side of the band correspond to high momentum transfer processes, right across the Fermi surface.

where the imaginary part determines the dissipative part of the magnetic response. The dissipation arises because an applied magnetic field generates a cloud of electron hole pairs which carry away the energy. If we use the Dirac-Cauchy relation $1/(x + i\delta) = P(1/x) - i\pi\delta(x)$ in (8.170), we obtain

$$\chi''(\mathbf{q}, \nu) = 2\mu_B^2 \int_{\mathbf{k}} \pi\delta[\nu - (\epsilon_{\mathbf{k+q}} - \epsilon_{\mathbf{k}})](f_{\mathbf{k}} - f_{\mathbf{k+q}}), \tag{8.174}$$

This quantity defines the density of states of particle-hole excitations. The excitation energy of a particle hole pair is given by

$$\epsilon_{\mathbf{k+q}} - \epsilon_{\mathbf{k}} = \frac{q^2}{2m} + \frac{qk}{m}\cos\theta$$

where θ is the angle between $\mathbf{k}$ and $\mathbf{q}$. This quantity is largest when $\theta = 0, k = k_F$ and smallest when $\theta = \pi, k = k_F$ so that

$$\frac{q^2}{2m} + \frac{qk_F}{m} > \nu > \frac{q^2}{2m} - \frac{qk_F}{m}$$

defines a band of allowed wavevectors where the particle-hole density of states is finite, as shown in Figure 8.5. Outside this region, $\chi_o(\mathbf{q}, \nu)$ is purely real.

8.6.2 Derivation of Lindhard Function

The dynamic spin-susceptibility

$$\chi(\mathbf{q},\nu) = 2\mu_B^2 \int_{\mathbf{k}} \frac{f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}}{(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - \nu)}. \tag{8.175}$$

can be rewritten as

$$\chi(\mathbf{q},\nu) = 2\mu_B^2 \int_{\mathbf{k}} f_{\mathbf{k}} \left[\frac{1}{(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - \nu)} + \frac{1}{(\epsilon_{\mathbf{k}-\mathbf{q}} - \epsilon_{\mathbf{k}} + \nu)} \right] \tag{8.176}$$

Written out explicity, this is

$$\chi(\mathbf{q},\nu) = 2\mu_B^2 \int_0^{k_F} \frac{k^2 dk}{2\pi^2} \int_{-1}^{1} \frac{d\cos\theta}{2} \left[\frac{1}{(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - \nu)} + ((\nu,\ \mathbf{q}) \to -(\nu,\ \mathbf{q})) \right].$$

By replacing $\epsilon_{\mathbf{k}} \to \frac{k^2}{2m} - \mu$ rescaling $x = k/k_F$, $\tilde{q} = q/(2k_F)$ and $\tilde{\nu} = \nu/(4\epsilon_F)$, we obtain $\chi(\mathbf{q},\nu) = \mu_B^2 N(0) \mathcal{F}(\tilde{q},\tilde{\nu})$, where

$$\mathcal{F}(\tilde{q},\tilde{\nu}) = \frac{1}{4\tilde{q}} \int_0^1 x^2 dx \int_{-1}^{1} dc \left[\frac{1}{xc + \tilde{q} - \frac{\tilde{\nu}}{\tilde{q}}} + (\nu \to -\nu) \right] \tag{8.177}$$

is the "Lindhard Function". Carrying out the integral over angle, we obtain

$$\begin{aligned} \mathcal{F}(\tilde{q},\tilde{\nu}) &= \frac{1}{4\tilde{q}} \int_0^1 x dx \left(\ln\left[\frac{\tilde{q} - \frac{\tilde{\nu}}{\tilde{q}} + x}{\tilde{q} - \frac{\tilde{\nu}}{\tilde{q}} - x} \right] + (\tilde{\nu} \to -\tilde{\nu}) \right) \\ &= \frac{1}{8\tilde{q}} \left(\left[1 - \left(\tilde{q} - \frac{\tilde{\nu}}{\tilde{q}} \right)^2 \right] \ln\left[\frac{\tilde{q} - \frac{\tilde{\nu}}{\tilde{q}} + 1}{\tilde{q} - \frac{\tilde{\nu}}{\tilde{q}} - 1} \right] + (\tilde{\nu} \to -\tilde{\nu}) \right) + \frac{1}{2} \end{aligned} \tag{8.178}$$

This function is known as the Lindhard function. Its static limit, $F(\tilde{q}) = \mathcal{F}(\tilde{q},\tilde{\nu}=0)$,

$$F(\tilde{q}) = \frac{1}{4\tilde{q}} \left(\left[1 - \tilde{q}^2 \right] \ln\left| \frac{\tilde{q}+1}{\tilde{q}-1} \right| \right) + \frac{1}{2} \tag{8.179}$$

has the property that $F(0) = 1$, and that dF/dx is singular at $x = 1$ as shown in Fig. 8.4. The imaginary part of $\chi(\mathbf{q}, \nu + i\delta)$ is given

$$\chi''(\mathbf{q},\nu) = \mu_B^2 N(0) \times \frac{\pi}{8\tilde{q}} \left\{ \left(1 - \left[\tilde{q} - \frac{\tilde{\nu}}{\tilde{q}} \right]^2 \right) \theta\left[1 - \left[\tilde{q} - \frac{\tilde{\nu}}{\tilde{q}} \right]^2 \right] - (\nu \to -\nu) \right\} \tag{8.180}$$

which is plotted in Fig. 8.5.

8.7 The RPA (Large-N) electron gas

Although the Feynman diagram approach gives us a way to generate all perturbative corrections, we still need a way to selecting the physically important diagrams. In general, as we have seen from the last examples, it is important to resum particular classes of diagrams to obtain a physical result. What principles can be used to select classes of diagrams?

Frequently however, there is no obvious choice of small parameter, in which case, one needs an alternative strategy. For example, in the electron gas, we could select diagrams according to the power of r_s entering the diagram. This would give us a high-density expansion of the properties - but what if we would like to examine a low density electron gas in a controlled way?

One way to select Feynman diagrams in a system with no natural small parameter is to take the so-called "large-N" limit. This involves generalizing some internal degree of freedom so that it has N components. Examples include:

- The Hydrogen atom in N-dimensions.
- The electron gas with $N = 2S + 1$ spin components.
- Spin systems, with spin S in the limit that S becomes large.
- Quantum Chromodynamics, with N, rather than three colours.

In each of these cases, the limit $N \to \infty$ corresponds to a new kind of semiclassical limit, where certain variables cease to undergo quantum fluctuations. The parameter $1/N$ plays the role of an effective $\hbar$

$$\frac{1}{N} \sim \hbar \tag{8.181}$$

This does not however mean that quantum effects have been lost, merely that their macroscopic consequences can be lumped into certain semi-classical variables.

8.7.1 The RPA electron gas

We shall now examine the second of these two examples. The idea is to take an interacting Fermi gas where each fermion has $N = 2S + 1$ possible spin components. The interacting Hamiltonian is still written

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2} \sum V_{\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma} \tag{8.182}$$

but now, the spin summations run over $N = 2S + 1$ values, rather than just two. As N is made very large, it is important that both the kinetic and the interaction energy scale extensively with N, and for this reason, the original interaction $V_{\mathbf{q}}$ is rescaled, writing

$$V_{\mathbf{q}} = \frac{1}{N} \mathcal{V}_{\mathbf{q}} \tag{8.183}$$

where it is understood that as $N \to \infty$, V is to be kept fixed. The idea is to now calculate quantities as an expansion in powers of $1/N$, and at the end of the calculation, to give N the value of specific interest, in our case, $N = 2$. For example, if we are interested in a Coulomb gas of spin $1/2$ electrons, then study the family of problems where

$$V_{\mathbf{q}} = \frac{1}{N}\frac{\tilde{e}^2}{q^2} = \frac{\mathcal{V}_{\mathbf{q}}}{N} \tag{8.184}$$

and $\tilde{e}^2 = 2e^2/\epsilon_0$. At the end, we set $N = 2$, boldly hoping that the key features of the solution around $N = 2$ will be shared by the entire family of models. In practice, this only holds true if the density of electron gas is large high enough to avoid instabilities, such as the formation of the Wigner crystal. For historical reasons, the approxation that appears in the large N limit is called the "Random Phase approximation" or "RPA" for short, a method developed during the 1950s. The early version of the RPA approximation was developed by Bohm and Pines[5] while its reformulation in a diagrammatic language was later given by Hubbard[6]. [2]. The large N treatment of the electron gas recovers RPA electron gas in a controlled approximation.

With the above substitution, the Feynman rules are unchanged, excepting that now we associate a factor $1/N$ with each interaction vertex. Before we start however, there are a few few preliminaries, in particular, we need to know how to handle long range Coulomb interactions. We'll begin considering a general $\tilde{V}_{\mathbf{q}}$ with a finite interaction range. To be concrete, we can consider a screened Coulomb interaction

$$\mathcal{V}_{\mathbf{q}} = \frac{\tilde{e}^2}{q^2 + \delta^2} \tag{8.185}$$

where we take $\delta \to 0$ at the end of the calculation to deal with the infinite range interaction.

8.7.2 Jellium: introducing an inert positive background.

To deal with long-range Coulomb interactions (and take $\delta \to 0$ in the above interaction (8.185)), we will need to make sure that the charge of the entire system is actually neutral. The resulting medium is a radically simplified version of matter that is playfully refered to as "jellium". In jellium, there is an inert and completely uniform background of positive charges, with charge $+|e|$ and number density $\rho_+(x) = \rho_+$ adjusted so that $\rho_+ = \rho_e$, the density of electrons. The the Coulomb interaction Hamiltonian of jellium takes the form

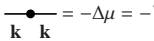
$$H_I = \frac{1}{2}\int_{\vec{x},\vec{y}} V(x-y) : (\hat{\rho}(x) - \rho_+)(\hat{\rho}(y) - \rho_+) := \frac{1}{2}\int_{\vec{x},\vec{y}} V(x-y) : \delta\rho(x)\delta\rho(y) : \tag{8.186}$$

where $\hat{\rho}(x)$ is the density of electrons and $\delta\rho(x) = \hat{\rho}(x) - \rho_+$ is the fluctuation of the density. We see that the Coulomb energy of jellium is only sensitive to the fluctuations in the density. The presence of the background charge has the the effect of upwardly shifting the chemical potential of the electrons by an amount

$$\Delta\mu = \int V(x-x')\rho_+(x') = V_{\mathbf{q}=0}\rho_+ \tag{8.187}$$

[2] A more detailed discussion of this early history can be found in the book by Nozières and Pines[7]

This chemical potential shift can be treated as a scattering potential that is diagonal in momentum, $\Delta V_{\mathbf{k},\mathbf{k}'} = -\Delta\mu\delta_{\mathbf{k},\mathbf{k}'}$, which introduces an additional uniform potential scattering term into the electron self energy



$$= -\Delta\mu = -V_{\mathbf{q}=0}\rho_+. \tag{8.188}$$

If we compare this term with the the "tadpole" diagrams in the self-energy

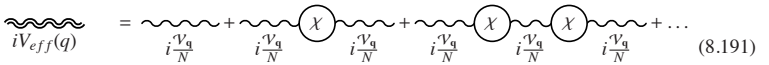
$$= -i(2S+1)V_{\mathbf{q}=0}\int_k G(k) = V_{\mathbf{q}=0}\rho_e. \tag{8.189}$$

we see that when we combine the terms, provided $\rho_e = \rho_+$, they cancel one-another.

$$= V_{\mathbf{q}}(\rho_e - \rho_+) = 0. \tag{8.190}$$

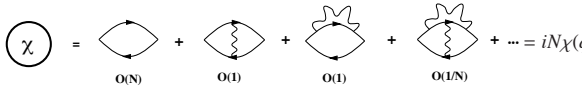
Thus by introducing a uniform positively charged background, we can entirely remove all tadpole insertions from the diagrams we draw.

Let us now examine how the fermions interact in this large-N fermi gas. We can expand the effective interaction as follows



(8.191)

The "self-energy" diagram for the interaction line is called a "polarization bubble", and has the following diagramatic expansion.



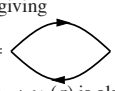
(8.192)

By summing the geometric series that appears in (8.191) we obtain

$$V_{eff} = \frac{1}{N}\frac{\mathcal{V}(q)}{1 + \mathcal{V}(q)\chi(q)} \tag{8.193}$$

This modification of the interaction by the polarization of the medium is an example of "screening". In the large-N limit, the higher-order Feynman diagrams for $\chi(q)$ are smaller by factors of $1/N$, so in the large-N limit, these terms can be neglected giving

$$i\chi(q)N = i\chi_0(q)N + O(1) =$$



$$+ O(1) \tag{8.194}$$

The large N approximation where we replace $\chi(q) \to \chi_0(q)$ is also called the "RPA appoximation".

In the case of a Coulomb interaction, where the screened interaction becomes

$$V_{eff}(\mathbf{q},\omega) = \frac{1}{N}\frac{\tilde{e}^2}{q^2\epsilon_{RPA}(\mathbf{q},\omega)} \tag{8.195}$$

where we have identified

$$\epsilon_{RPA}(\mathbf{q},\omega) = 1 + \mathcal{V}(q)\chi(q) = 1 + \frac{\tilde{e}^2}{q^2}\chi_o(q) \tag{8.196}$$

as the dielectric function of the charged medium. Notice how, in the interacting medium, the interaction between the fermions has become frequency dependent, indicating that the interactions between the particles are now *retarded*. From our previous study of the Linhard function, we showed that $\chi_o(q) = N_s(0)\mathcal{F}(q/(2k_F)), \nu/(4\epsilon_F))$ where $\mathcal{F}$ is the dimensionless Lindhard function and $N_s(0) = \frac{mk_F}{2\pi^2\hbar^2}$ is the density of states per spin at the Fermi surface, so we may write

$$\epsilon_{RPA}(\mathbf{q},\omega) = 1 + \lambda\left(\frac{\mathcal{F}(\tilde{q},\tilde{\nu})}{\tilde{q}^2}\right) \tag{8.197}$$

where the dimensionless coupling constant

$$\lambda = \frac{\tilde{e}^2 N_s(0)}{(2k_F)^2} = \frac{1}{\pi k_F}\times\frac{e^2 m}{4\pi\epsilon_0\hbar^2} = \frac{1}{\pi k_F a_B} = \left(\frac{\alpha}{\pi}\right)r_s, \tag{8.198}$$

here a_B is the Bohr radius $\alpha = \left(\frac{4}{9\pi}\right)^{1/3} \approx 0.521$ and $r_s = (\alpha k_F a_B)^{-1}$ is the dimensionless electron separation (see 8.105). Notice that the accuracy of the large N expansion places no restriction on the size of the coupling constant λ, which may take any value in the large N limit. Summarizing,

$$\epsilon_{RPA}(\mathbf{q},\omega) = 1 + \frac{1}{\pi k_F a_B}\left(\frac{\mathcal{F}(\tilde{q},\tilde{\nu})}{\tilde{q}^2}\right) \tag{8.199}$$

Dielectric constant of the RPA electron gas

8.7.3 Screening and Plasma oscillations

At zero frequency and low momentum, $\mathcal{F} \to 1$, so the dielectric constant diverges:

$$\epsilon = \lim_{q\to 0}\epsilon(\mathbf{q},\nu=0) \to \infty.$$

Is this a failure of our theory?

In fact: no! The divergence of the uniform, static dielectric constant is the quintisential electrostatic property of a metal. Since $\epsilon = \infty$, no static electric fields penetrate a metal. Moreover, the electron charge is completely screened. At small q, the effective interaction is

$$V_{eff}(\mathbf{q},\nu) = \frac{1}{N}\frac{\tilde{e}^2}{q^2+\kappa^2} \equiv \frac{e^2}{\epsilon_0(q^2+\kappa^2)}, \qquad (N=2) \tag{8.200}$$

where $\kappa = \sqrt{\tilde{e}^2 N_s(o)} = \sqrt{e^2 N(0)/\epsilon_0}$ $(N=2)$ can be identified as an inverse screening length. κ^{-1} is the "Thomas-Fermi" screening length of a classical charge plasma. You can think of

$$e_{screening}(q) = \frac{e}{\epsilon(\mathbf{q},0)} - e \sim |e|\frac{\kappa^2}{q^2+\kappa^2}$$

(where $e = -|e|$), as the Fourier transform of the screening charge around the electron. We can see that the electron charge is fully screened, since $e_{screening}(q=0) = +|e|$. Note however, that there is still a weak singularity in the susceptibility when $q \sim 2k_F$, $\chi_0(q\sim 2k_F, 0) \sim (q-2k_F)\ln(q-2k_F)$, which Fourier transformed, gives rise to a long-range *oscillatory* component to the interaction between the particles of the form

$$V_{eff}(r) \propto \frac{\cos 2k_F r}{r^3}. \tag{8.201}$$

This long-range oscillatory interaction is associated with Friedel oscillations.

A second, and related consequence of the screening is the emergence collective of plasma oscillations. In the opposite limit of finite frequency, but low momentum, we may approximate χ_0 by expanding it in momentum, as follows

$$\chi_o(\mathbf{q},\nu) = \int_{\mathbf{k}}\frac{f_{\mathbf{k}+\mathbf{q}} - f_{\mathbf{k}}}{\nu - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})} \approx \int_{\mathbf{k}}\frac{(\mathbf{q}\cdot\mathbf{v}_{\mathbf{k}})}{\nu - (\mathbf{q}\cdot\mathbf{v}_{\mathbf{k}})}\left(\frac{df(\epsilon)}{d\epsilon}\right) \tag{8.202}$$

where $\mathbf{v}_{\mathbf{k}} = \nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}$ is the group velocity. Expanding this to leading order in momentum gives

$$\chi_o(\mathbf{q},\nu) = -\int_{\mathbf{k}}\frac{(\mathbf{q}\cdot\mathbf{v}_{\mathbf{k}})^2}{\nu^2}\left(-\frac{df(\epsilon)}{d\epsilon}\right) = -\frac{N_s(0)v_F^2}{3}\left(\frac{q^2}{\nu^2}\right) = -\left(\frac{\tilde{n}}{m}\right)\left(\frac{q^2}{\nu^2}\right), \tag{8.203}$$

where $\tilde{n} = n/N$ is the density of electrons per spin, so that

$$\epsilon_o(\mathbf{q},\nu) = 1 - \frac{\omega_p^2}{\nu^2} \tag{8.204}$$

where

$$\omega_p^2 = \frac{\tilde{e}^2\tilde{n}}{m} = \frac{e^2 n}{\epsilon_0 m} \qquad (N=2). \tag{8.205}$$

is the plasma frequency. This zero in the dielectric function at $\omega = \omega_p$ indicates the presence of collective plasma oscillations in the medium at frequency ω_p. At finite q, $\omega_P(q)$ develops a, forming a collective mode.

It is instructive to examine the response of the electron gas to a time-dependent change in potential energy $-\delta U(x,t)$ (corresponding to a change in energy $H = -\int\delta U(x,t)\rho(x)$) with Fourier transform $\delta U(q)$. In a non-interacting electron gas, the induced change in charge is

$$\delta\rho_e(q) = N_s\chi_0(q)\delta U(q)$$

corresponding to the diagram

$$\delta\rho_e(q) = -i \quad \delta U(q) \tag{8.206}$$

In the RPA electron gas, the change in the electron density induced by the applied potential produces its own interaction, and the induced change in charge is given by

$$\begin{aligned}\delta\rho_e(q) &= -i\Big[+ + + \ldots \Big]\delta U(q) \\ &= N\Big[\chi_0 + \chi_0(-\mathcal{V}\chi_0) + \chi_0(-\mathcal{V}\chi_0)^2 + \ldots\Big]\delta U(q) \\ &= N\left[\frac{\chi_0(q)}{1+\mathcal{V}_q\chi_0(q)}\right]\delta U(q).\end{aligned} \tag{8.207}$$

So we see that the dynamical charge susceptibility is renormalized by interactions

$$\chi(q) = N\frac{\chi_0(q)}{\epsilon_{RPA}(q)} = N(0)\left[\frac{\mathcal{F}(\tilde{q},\tilde{\nu})}{1+\frac{\alpha r_s}{\pi}\mathcal{F}(\tilde{q},\tilde{\nu})}\right], \qquad (\tilde{q} = q/2k_F,\ \tilde{\nu} = \nu/4\epsilon_F) \tag{8.208}$$

where $\mathcal{F}(\tilde{q},\tilde{\nu})$ is given in (8.178). The imaginary part of the dynaical susceptibility $\chi(\mathbf{q}, \nu - i\delta)$ defines the spectrum of collective excitations of the RPA electron gas, shown in in Fig. 8.6. Notice how the collective plasma mode is split off above the particle-hole continuum.

Remarks:

- The appearance of this plasma mode depends on the singular, long-range nature of the Coulomb interaction. It is rather interesting to reflect on what would have happened to the results of this section had we kept the regulating δ in the bare interaction $\mathcal{V}_q$ (8.185) finite. In this case the plasma frequency would be zero, while the dielectic constant would be finite. In other words, the appearance of the plasma mode, and the screening of an infinite range interaction are intimately interwined. In fact, the plasma mode in the Coulomb gas is an elementary example of a Higg's particle - a finite mass excitation that results from the screening of a long-range (gauge) interaction. We shall discuss this topic in more depth in section (**??**).

8.7.4 Zero point energy of the RPA electron gas.

Let us now examine the linked cluster expansion of the ground-state energy. Without the tadpole insertions, the only non-zero diagrams are then:

$$\frac{\Delta E}{V} = \Big(+ + + \ldots \Big)$$

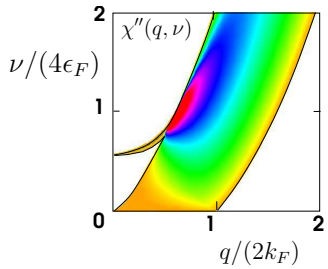


Figure 8.6: Density plot of the imaginary part of the dynamical charge susceptibility $Im[\chi_0(\mathbf{q},\nu)/\epsilon(\mathbf{q},\nu)]$ in the presence of the Coulomb interaction calculated for $\frac{\alpha r_s}{\pi} = 1$, ($r_s \sim 6$). using eq. (8.199) and eq. (8.178). Notice the split-off plasmon frequency mode, and how the charge fluctuations have moved up to frequencies above the plasma frequency.

$$+ \left(+ \quad \text{O(1/N)} \quad +\ldots \right) + \left(\quad \text{O(1/N}^2\text{)} \quad +\ldots \right) + \ldots \ldots \Big] \tag{8.209}$$

These diagrams are derived from the zero the zero-point fluctuations in charge density, which modify the ground-state energy $E \to E_o + E_{zp}$. We shall select the leading contribution

$$\frac{E_{zp}}{V} = + \quad \text{O(1)} \quad + \quad + \quad +\ldots \tag{8.210}$$

Now the *nth* diagram in this series has a symmetry factor $p = 2n$, and a contribution $(-\chi_o(q)\mathcal{V}(q))^n$ associated with the n polarization bubbles and interaction lines. The energy per unit volume associated with this series of diagrams is thus

$$E_{zp} = i\sum_{n=1}^{\infty}\frac{1}{2n}\int\frac{d^4q}{(2\pi)^4}(-\chi_o(q)\mathcal{V}(q))^n. \tag{8.211}$$

By interchanging the sum and the integral, we see that we obtain a series of the form $\sum_n \frac{(-x)^n}{n} = -\ln(1+x)$, so that the zero-point correction to the ground-state energy is

$$E_{zp} = -i\frac{1}{2}\int\frac{d^4q}{(2\pi)^4}ln[1+\mathcal{V}_{\mathbf{q}}\chi_o(q)]$$

Now the logarithm has a branch cut just below the real axis, for positive frequency, but just above the real axis for negative frequency. If we carry out the frequency integral by completing the contour in

the lower half plane, we can distort the contour integral around the branch cut at positive frequency, to obtain

$$\begin{aligned} E_{zp} &= -\frac{i}{2}\int_{\mathbf{q}}\int_0^\infty \frac{d\omega}{2\pi}\left[\ln[1+\chi_o(\mathbf{q},\nu+i\delta)\mathcal{V}_{\mathbf{q}}]-\ln[1+\chi_o(\mathbf{q},\nu-i\delta)\mathcal{V}_{\mathbf{q}}]\right] \\ &= \frac{1}{2}\int_{\mathbf{q}}\int_0^\infty \frac{d\omega}{\pi}\arctan\left(\frac{\mathcal{V}_{\mathbf{q}}\chi''(\mathbf{q},\nu)}{[1+\mathcal{V}_{\mathbf{q}}\chi'(\mathbf{q},\nu)]}\right) \end{aligned} \tag{8.212}$$

If we associate a "phase shift"

$$\delta(\mathbf{q},\omega) = \arctan\left(\frac{\mathcal{V}_{\mathbf{q}}\chi''(\mathbf{q},\nu)}{[1+\mathcal{V}_{\mathbf{q}}\chi'(\mathbf{q},\nu)]}\right) \tag{8.213}$$

then we can the zero-point fluctuation energy can also be written in the form

$$\Delta E_{zp} = \int \frac{d^3q}{(2\pi)^3}\int_0^\infty d\omega\Lambda(\omega)\left[\frac{\omega}{2}\right] \tag{8.214}$$

where

$$\Lambda(\omega) = \frac{1}{\pi}\frac{\partial\delta(\mathbf{q},\omega)}{\partial\omega}. \tag{8.215}$$

We can interpret $\Lambda(\omega)$ as the "density of states" of charge fluctuations at an energy ω. When the interactions are turned on, each charge fluctuation mode in the continuum experiences a scattering phase shift $\delta(\vec{q},\omega)$ which has the effect of changing the density of states of charge fluctuations. The zero-point energy describes the change in the energy of the continuum due to these scattering effects.

8.8 Exercises

1. The separation of electrons $R_e$in a Fermi gas is defined by

$$\frac{4\pi R_e^3}{3} = \rho^{-1}$$

where ρ is the density of electrons. The dimensionless separation r_s is defined as $r_s = R_e/a$ where $a = \frac{c\hbar^2}{me^2}$ is the Bohr radius.

(a) Show that the Fermi wavevector is given by

$$k_F = \frac{1}{\alpha r_s a}$$

where $\alpha = \left(\frac{4}{9\pi}\right)^{\frac{1}{3}} \approx 0.521$.

(b) Consider an electron plasma where the background charge density precisely cancels the charge density of the plasma. Show that the ground-state energy to leading order in the strength of the Coulomb interaction is given by

$$\begin{aligned} \frac{E}{\rho V} &= \frac{3}{5}\frac{R_Y}{\alpha^2 r_s^2} - \frac{3}{2\pi}\frac{R_Y}{\alpha r_s} \\ &= \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_S}\right)R_Y \end{aligned} \tag{8.216}$$

where $R_Y = \frac{\hbar^2}{2ma^2}$ is the Rydberg energy. (Hint - in the electron gas with a constant charge background, the Hartree part of the energy vanishes. The Fock part is the second term in this expression. You may find it useful to use the integral

$$\int_0^1 dx\int_0^1 dy xy\ln|\frac{x+y}{x-y}| = \frac{1}{2}$$

(c) When can the interaction effects be ignored relative the kinetic energy?

2. Consider a gas of particles with interaction

$$\hat{V} = 1/2\sum_{\vec{k}\vec{k}'\vec{q}\sigma\sigma'} V_q c^\dagger_{\vec{k}-\vec{q}\sigma} c^\dagger_{\vec{k}'+\vec{q}\sigma'} c_{\vec{k}'\sigma'} c_{\vec{k}\sigma}$$

(a) Let $|\phi\rangle$ represent a filled Fermi sea, i.e. the ground state of the non interacting problem. Use Wick's theorem to evaluate an expression for the expectation value of the interaction energy $\langle\phi|\hat{V}|\phi\rangle$ in the non-interacting ground state. Give a physical interpretation of the two terms that arise and draw the corresponding Feynman diagrams.

(b) Suppose $|\tilde{\phi}\rangle$ is the full ground-state of the interacting system. If we add the the interaction energy $\langle\tilde{\phi}|\hat{V}|\tilde{\phi}\rangle$ to the non-interacting ground-state energy, do we obtain the full ground-state energy? Please explain your answer.

(c) Draw the Feynman diagrams corresponding to the second order corrections to the ground-state energy. Without calculation, write out each diagram in terms of the electron propagators and interaction V_q, being careful about minus signs and overall pre-factors.

3. Consider a d-dimensional system of fermions with spin-degeneracy $N = 2S+1$, mass m and total density $N\rho$, where ρ is the density per spin component. The fermions attract one-another via the two-body potential

$$V(\mathbf{r}_i - \mathbf{r}_j) = -\alpha\delta^{(d)}(\mathbf{r}_i - \mathbf{r}_j), \qquad (\alpha > 0) \tag{8.217}$$

(a.) Calculate the *total* energy *per particle*, $\epsilon_s(N,\rho)$ to first order in α.

(b.) Beyond some critical value α_c, the attraction between to the particles becomes so great that the gas becomes unstable, and may collapse. Calculate the dependence of α_c on the density per spin ρ. To what extent do you expect the gas to collapse in $d = 1, 2, 3$ when α_c is exceeded?

(c.) In addition to the above two-body interaction nucleons are also thought to interact via a repulsive three-body interaction. Write the three-body potential $V(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k) = \beta\delta^{(d)}(\mathbf{r}_i - \mathbf{r}_j)\delta^{(d)}(\mathbf{r}_j - \mathbf{r}_k)$, in second-quantized form.

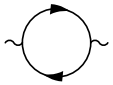
(d.) Use Feynman diagrams to calculate the ground-state energy *per particle*, $\epsilon_s(N,\rho)$ to leading order in both β and α. How does your result compare with that obtained in (a) when $N = 2$?

(e.) If we neglect Coulomb interactions, why is the case $N = 4$ relevant to nuclear matter?

4. (a.)Consider a system of fermions interacting via a momentum-dependent interaction $V(\mathbf{q}) = \frac{1}{N}U(\mathbf{q})$, where $N = 2S + 1$ is the spin degeneracy. When N is large, the interactions in this fluid can be treated exactly. Draw the Feynman diagram expansion for the ground-state energy, identifying the leading and subleading terms in the $1/N$ expansion.

   (b) Certain classes of Feynman diagrams in the linked-cluster expansion of the ground-state energy identically vanish. Which ones, and why?

   (c.) If $N\chi^{(o)}(q) = \langle \delta\rho(q)\delta\rho(-q)\rangle_o$ is the susceptibility of the non-interacting Fermi gas, i.e



$$= iN\chi^{(o)}(q), \tag{8.218}$$

   where $q = (\mathbf{q}, \nu)$, what is the effective interaction between the fermions in the large N limit? Suppose that in real space, $U(r) = e^2/r$ is a long-range Coulomb interaction, explain in detail what happens to the effective interaction at long-distances.

5. Compute the rms quantum fluctuations $\Delta\rho = \sqrt{\langle(\rho - \rho_o)^2\rangle}$ in the charge density of the electron gas about its average density, ρ_o, in the large-N limit. Show that $\Delta\rho/\rho_o \sim O(1/N)$, so that the density behaves as a semiclassical variable in the large N limit.

6. Show that the dynamical charge susceptibility of an interacting electron gas in the large N limit, defined by

$$\chi(\mathbf{q}, \nu + i\delta) = \int d^3x \int_0^\infty i\langle\phi|[\rho(\mathbf{x}, t), \rho(0, 0)]|\phi\rangle e^{-i(\mathbf{q}\cdot\mathbf{x} - \omega t)} \tag{8.219}$$

   contains a pole at frequencies

$$\omega_q = \omega_p(1 + \frac{3}{10}qv_F) \tag{8.220}$$

   where $\omega_p = \sqrt{4\pi e^2\tilde{n}/m}$ is the Plasma frequency and $v_F = p_F/m$ is the Fermi velocity.

Table. 8.1 Real Space Feynman Rules .

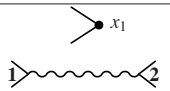
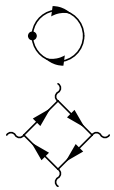
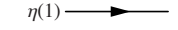
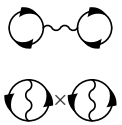
	$G(\mathbf{2} - \mathbf{1})$
	$U(x_1)$ $iV(\mathbf{1} - \mathbf{2})$
$\prod_i \int d^3x_i dt_i$	Integrate over all intermediate times and positions.
	$-(2S + 1)G(\vec{0}, 0^-)$ $[-(2S + 1)]^F$, F = no. Fermion loops.
	$\eta(1)$ $-i\bar{\eta}(1)$
	$p = 2$ $p = 8$ $\frac{1}{p}$ p = order of symmetry group.

Table. 8.2 Momentum Space Feynman Rules .

$(\mathbf{k},\omega)$	$G_o(\mathbf{k},\omega)$	Fermion propagator
1 2 $(\mathbf{q},\nu)$	$iV(q)$ $ig_q^2 D_o(q)$	Interaction Exchange Boson.
q	$U(\mathbf{q})$	Scattering potential
	$[-(2S+1)]^F$,	F= no. Fermion loops
$(\mathbf{q},\nu)$	$\int \frac{d^dq d\nu}{(2\pi)^{d+1}} e^{i\nu 0^+}$	Integrate over internal loop momenta and frequency.
$p=2$ $p=8$	$\frac{1}{p}$	p = order of symmetry group.

Table. 8.3 Relationship With Physical Quantities.

ΔE	$iV\sum\{\text{linked clusters}\}$	$iV\left[\quad + \quad + \ldots\right]$
$\ln S$	$VT\sum\{\text{linked clusters}\}$	$VT\left[\quad + \quad + \ldots\right]$
$1 \longrightarrow 2$ $-i\langle T\psi(2)\psi^\dagger(1)\rangle$	$\sum\{\text{Two leg diagrams}\}$	$\Sigma +$ + +
$(-i)^n\langle T\psi(1)\ldots\psi^\dagger(2n)\rangle$ G $n=2$	$\sum\{\text{2n- leg diagrams}\}$	$\Sigma \quad \Sigma$ $-$ + + χ $iV_{eff}(q)$ $i\frac{V_q}{N}$ $i\frac{V_q}{N}$ $i\frac{V_q}{N}$
Response Functions $(-i)^2\langle\psi\|T[A(2)B(1)]\|\psi\rangle = \chi^T_{AB}$ $B(1)$ $A(2)$ $i\langle[A(2),B(1)]\rangle\theta(t_1-t_2) = \chi_{AB}$	$\chi_{AB} = -i\chi^T_{AB}(\omega - i\delta)$	$-i\times$ + + …

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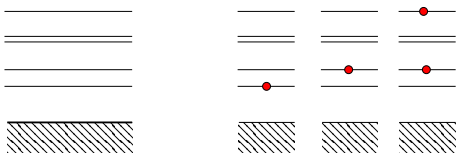
Chapter 9

Finite Temperature Many Body Physics

For most purposes in many body theory, we need to know how to include the effects of temperature. At first sight, this might be thought to lead to undue extra complexity in the mathematics, for now we need to average the quantum effects over an ensemble of states, weighted with the Boltzmann average

$$p_\lambda = \frac{e^{-\beta E_\lambda}}{Z} \tag{9.1}$$

It is here that some of the the most profound aspects of many body physics come to our aid.



Ground State T=0 Ensemble of states at temperature T> 0

$$p_\lambda = \frac{e^{-\beta E_\lambda}}{Z}$$

Figure 9.1: At zero temperature, the properties of a system are determined by the ground-state. At finite temperature, we must average the properties of the system over an ensemble which includes the ground-state and excited states, averaged with the Boltzmann probability weight $\frac{e^{-\beta E_\lambda}}{Z}$.

Remarkably, finite temperature Many Body physics is no more difficult than its zero temperature partner, and in many ways, the formulation is easier to handle. The essential step that makes this possible is due to the Japanese physicist Kubo, who noticed in the early fifties that the quantum-mechanical partition function can be regarded as a time-evolution operator in *imaginary time*:

$$\hat{\rho} \propto e^{-\beta \hat{H}} = U(-i\hbar\beta),$$

where $U(t) = e^{-i\frac{tH}{\hbar}}$ is the time-evolution operator, and by convention, we write $H = H_0 - \mu N$ to take into account of the chemical potential. Kubo's observation led him to realize that finite temperature many body physics can be compactly reformulated using an imaginary, rather than a real time to time-evolve all states

$$\frac{it}{\hbar} \longrightarrow \tau.$$

Kubo's observation was picked up by Matsubara, who wrote down the first imaginary time formulation of finite temperature many body physics. In the imaginary time approach, the partition function of a quantum system is simply the trace of the time-evolution operator, evaluated at imaginary time t = -i $\hbar\beta$,

$$Z = Tre^{-\beta H} = TrU(-i\hbar\beta),$$

whilst the expectation value of a quantity A in thermal equilibrium is given by

$$\langle A\rangle = \frac{Tr\left[U(-i\hbar\beta)A\right]}{Tr\left[U(-i\hbar\beta)\right]},$$

an expression reminiscent of the Gell-Mann Lowe formula excepting that now, the S-matrix is replaced by time-evolution over the *finite* interval $t \in [0, -i\hbar\beta]$: The imaginary time universe is of finite extent in the time direction! We will see that physical quantities turn out to be periodic in imaginary time, over this finite interval $\tau \in [0, \hbar\beta]$. This can loosely understood as a consequence of the incoherence induced by thermal fluctuations: thermal fluctuations lead to an uncertainty k_BT in energies, so

$$\tau_T = \frac{\hbar}{k_BT}$$

represents a characteristic time of a thermal fluctuation. Processes of duration longer than τ_T loose their phase coherence, so coherent quantum processes are limited within a world of finite temporal extent, $\hbar\beta$.

One of the most valuable aspects of finite temperature quantum mechanics, first explored by Kubo concerns the intimate relationship between response functions and correlation functions in both real and imaginary time, which are mathematically quantified via the "fluctuation dissipation theorem".

Quantum/thermal Fluctuations ↔ Dynamic Response

"Fluctuation dissipation"

These relationships, first exploited in detail by Kubo, and now known as the "Kubo formalism", enable us to calculate correlation functions in imaginary time, and then, by analytically continuing the Fourier spectrum, to obtain the real-time response and correlation functions at a finite temperature.

Most theoretical many body physics is conducted in the imaginary time formalism, and theorists rarely give the use of this wonderful method a moments use. It is probably fair to say that we do

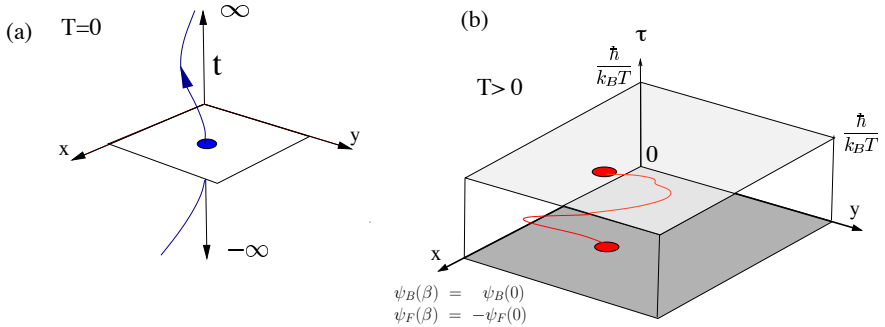


Figure 9.2: (a) Zero temperature field theory is carried out in a space that extends infinitely from $t = -\infty$ to $t = \infty$. (b) Finite temperature field theory is carried out in a space that extends over a finite time, from $\tau = 0$ to $\tau = \hbar\beta$. Bosonic fields (ψ_B) are periodic over this interval whereas Fermionic fields (ψ_F) are antiperiodic over this interval.

not understand the deep reasons why the imaginary time formalism works. Feynman admits in his book on Statistical mechanics, that he has sought, but not found a reason for why imaginary time and thermal equilibrium are so intimately intertwined. In relativity, it turns out that thermal density matrices are always generated in the presence of an event horizon, which excludes any transmission of information between the halves of the universe of different sides of the horizon. It would seem that a complete understanding of imaginary time may be bound-up with a more complete understanding of information theory and quantum mechanics than we currently possess. What-ever the reason, it is a very pragmatic and beautiful approach, and it is this which motivates us to explore it further!

9.1 Imaginary time

The key step in making the jump from zero temperature, to finite temperatures many body physics, is the replacement

$$\frac{it}{\hbar} \to \tau. \tag{9.2}$$

With this single generalization, we can generalize almost everything we have done at zero tem-

perature. In zero temperature quantum mechanics, we introduced the idea of the Schrödinger, Heisenberg and interaction representations. We went on to introduce the concept of the Greens function, and developed a Feynman diagram expansion of the S-matrix. We shall now repeat this exact procedure in imaginary time, reinterpreting the various entities which appear in terms of finite temperature statistical mechanics. Table 1. summarizes the key analogies between real time zero temperature, and imaginary time, finite temperature many body physics.

Table. 9.0 The link between real and imaginary time formalisms.

Schrödinger eqn	$\|\psi_s(t)\rangle = e^{-itH}\|\psi_s(0)\rangle$	$\|\psi_s(\tau)\rangle = e^{-\tau H}\|\psi_s(0)\rangle$
Heisenberg rep	$A_h = e^{itH}A_s e^{-itH}$	$A_H = e^{\tau H}A_s e^{-\tau H}$
Interaction rep	$\|\psi_I(t)\rangle = e^{-itH_0}\|\psi_I(t)\rangle$	$\|\psi_I(\tau)\rangle = e^{-\tau H_0}\|\psi_I(\tau)\rangle$
Perturbation Expansion	$S = \langle -\infty\|Te^{-i\int Vdt}\|\infty\rangle$	$\frac{Z}{Z_0} = Tr\left[e^{-\int_0^\beta Vd\tau}\right]$
Wick's Theorem	$\overbrace{\psi(1)\psi^\dagger(2)} = \langle 0\|T\psi(1)\psi^\dagger(2)\|0\rangle$	$\overbrace{\psi(1)\psi^\dagger(2)} = \langle T\psi(1)\psi^\dagger(2)\rangle$
Green's function	$G_{\lambda\lambda'}(t) = -i\langle 0\|T\psi_\lambda(\tau)\psi^\dagger{}_{\lambda'}(0)\|0\rangle$	$\mathcal{G}_{\lambda\lambda'}(\tau) = -\langle T\psi_\lambda(\tau)\psi^\dagger{}_{\lambda'}(0)\rangle$
Feynman Diagrams	$\ln S = TV\sum$[linked clusters] $= -iT\Delta E$	$\ln\frac{Z}{Z_o} = \beta V\sum$[linked clusters] $= -\beta\Delta F$

9.1.1 Representations

The imaginary time generalization of the Heisenberg and interaction representations precisely parallels the development in real time, but there are some minor differences that require us to go through the details here. After making the substitution $t \to -i\tau\hbar$, the real time Schrödinger equation

$$H|\psi_s\rangle = i\hbar\frac{\partial}{\partial t}|\psi_s\rangle, \tag{9.3}$$

becomes

$$H|\psi_s\rangle = -\frac{\partial}{\partial\tau}|\psi_s\rangle. \tag{9.4}$$

so the time-evolved wavefunction is given by

$$|\psi_s(\tau)\rangle = e^{-H\tau}|\psi_s(0)\rangle. \tag{9.5}$$

The Heisenberg representation removes all time-dependence from the wavefunction, so that $|\psi_H\rangle = |\psi_s(0)\rangle$ and all time-evolution is transfered to the operators,

$$A_H(\tau) = e^{iH(-i\tau)}A_S e^{-iH(-i\tau)} = e^{H\tau}A_S e^{-H\tau}. \tag{9.6}$$

so that the Heisenberg equation of motion becomes

$$\frac{\partial A_H}{\partial \tau} = [H, A_H]$$

If we apply this to the free particle Hamiltonian

$$H = \sum \epsilon_k c^\dagger{}_k c_k$$

we obtain

$$\begin{aligned} \frac{\partial c_k}{\partial \tau} &= [H, c_k] = -\epsilon_k c_k \\ \frac{\partial c^\dagger{}_k}{\partial \tau} &= [H, c^\dagger{}_k] = \epsilon_k c^\dagger{}_k \end{aligned} \tag{9.7}$$

so that

$$\left.\begin{aligned} c_k(\tau) &= e^{-\epsilon_k\tau}c_k \\ c^\dagger{}_k(\tau) &= e^{\epsilon_k\tau}c^\dagger{}_k \end{aligned}\right\} \quad \text{(p.s} \quad c^\dagger{}_k(\tau) = (c_k(-\tau))^\dagger \neq (c_k(\tau))^\dagger \quad \text{)}. \tag{9.8}$$

Notice a key difference to the real-time formalism: in the imaginary time Heisenberg representation, creation and annihilation operator are no longer Hermitian conjugates.

We go on next, to develop the Interaction representation, which freezes time-evolution from the non-interacting part of the Hamiltonian H_0, so that

$$|\psi_I(\tau)\rangle = e^{H_0\tau}|\psi_s(\tau)\rangle = e^{H_0\tau}e^{-H\tau}|\psi_H\rangle = U(\tau)|\psi_H\rangle$$

where $U(\tau) = e^{H_0\tau}e^{-H\tau}$ is the time evolution operator. The relationship between the Heisenberg and the interaction representation of operators is given by

$$A_H(\tau) = e^{H\tau}A_S e^{-H\tau} = U^{-1}(\tau)A_I(\tau)U(\tau)$$

In the interaction representation, states can be evolved between two times as follows

$$|\psi_I(\tau_1)\rangle = U(\tau_1)U^{-1}(\tau_2))|\psi_I(\tau_2)\rangle = S(\tau_1,\tau_2)|\psi_I(\tau_2)\rangle$$

The equation of motion for $U(\tau)$ is given by

$$\begin{aligned} -\frac{\partial}{\partial\tau}U(\tau) &= -\frac{\partial}{\partial\tau}\left[e^{H_o\tau}e^{-H\tau}\right] \\ &= e^{H_o\tau}Ve^{-H\tau} \\ &= e^{H_o\tau}Ve^{-H_o\tau}U(\tau) \\ &= V_I(\tau)U(\tau) \end{aligned} \tag{9.9}$$

and a similar equation applies to $S(\tau_1,\tau_2)$,

$$-\frac{\partial}{\partial\tau}S(\tau_1,\tau_2) = V_I(\tau_1)S(\tau_1,\tau_2). \tag{9.10}$$

These equations parallel those in real time, and following exactly analogous procedures, we deduce that the imaginary time evolution operator in the interaction representation is given by a time-ordered exponential, as follows

$$\begin{aligned} U(\tau) &= T\exp\left[-\int_0^\tau V_I(\tau)d\tau\right] \\ S(\tau_1,\tau_2) &= T\exp\left[-\int_{\tau_1}^{\tau_2} V_I(\tau)d\tau\right]. \end{aligned} \tag{9.11}$$

One of the immediate applications of these results, is to provide a perturbation expansion for the partition function. We can relate the partition function to the time-evolution operator in the interaction representation as follows

$$\begin{aligned} Z &= \mathrm{Tr}\left[e^{-\beta H}\right] = \mathrm{Tr}\left[e^{-\beta H_o}U(\beta)\right] \\ &= \overbrace{\mathrm{Tr}\left[e^{-\beta H_0}\right]}^{Z_0}\overbrace{\left(\frac{\mathrm{Tr}\left[e^{-\beta H_o}U(\beta)\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]}\right)}^{\langle U(\beta)\rangle_0} \\ &= Z_0\langle U(\beta)\rangle_0 \end{aligned} \tag{9.12}$$

enabling us to write the ratio of the interacting, to the non-interacting partition function as the expectation value of the time-ordered exponential in the non-interacting system.

$$\frac{Z}{Z_0} = e^{-\beta\Delta F} = \langle T\exp\left[-\int_0^\beta V_I(\tau)d\tau\right]\rangle \tag{9.13}$$

Notice how the logarithm of this expression gives the shift in Free energy resulting from interactions. The perturbative expansion of this relation in powers of V is basis for the finite temperature Feynman diagram approach.

9.2 Imaginary Time Green Functions

The finite temperature Green function is defined to be

$$\mathcal{G}_{\lambda\lambda'}(\tau-\tau') = -\langle T\psi_\lambda(\tau)\psi_{\lambda'}{}^\dagger(\tau')\rangle = -Tr\left[e^{-\beta(H-F)}\psi_\lambda(\tau)\psi_{\lambda'}{}^\dagger(\tau')\right] \tag{9.14}$$

where ψ_λ can be either a fermionic or bosonic field, evaluated in the Heisenberg representation, $F = -T\ln Z$ is the Free energy. The T inside the angle brackets the time-ordering operator. Provided

H is time independent, time-translational invariance insures that $\mathcal{G}$ is solely a function of the time difference $\tau-\tau'$. In most cases, we will refer to situations where the quantum number λ is conserved, which will permit us to write

$$\mathcal{G}_{\lambda\lambda'}(\tau) = \delta_{\lambda\lambda'}\mathcal{G}_{\lambda}(\tau).$$

For the case of continuous quantum numbers λ, such as momentum, it is convention to promote the quantum number into the argument of the Green function, writing $\mathcal{G}(\mathbf{p},\tau)$ rather than $\mathcal{G}_{\mathbf{p}}(\tau)$.

As an example, consider a non-interacting system with Hamiltonian

$$H = \sum \epsilon_\lambda \psi^\dagger{}_\lambda \psi_\lambda, \tag{9.15}$$

where $\epsilon_\lambda = E_\lambda - \mu$ is the one-particle energy, shifted by the chemical potential. Here, the equal time expectation value of the fields is

$$\langle \psi_{\lambda'}{}^\dagger \psi_\lambda\rangle = \delta_{\lambda\lambda'}\left\{\begin{array}{ll} n(\epsilon_\lambda) & \text{(Bosons)} \\ f(\epsilon_\lambda) & \text{(Fermions)}\end{array}\right. \tag{9.16}$$

where

$$\begin{aligned} n(\epsilon_\lambda) &= \frac{1}{e^{\beta\epsilon_\lambda}-1} \\ f(\epsilon_\lambda) &= \frac{1}{e^{\beta\epsilon_\lambda}+1}\end{aligned} \tag{9.17}$$

are the Bose and Fermi functions respectively. Similarly,

$$\langle \psi_\lambda \psi^\dagger{}_{\lambda'}\rangle = \delta_{\lambda\lambda'} \pm \langle \psi_{\lambda'}{}^\dagger \psi_\lambda\rangle = \delta_{\lambda\lambda'}\left\{\begin{array}{ll} 1+n(\epsilon_\lambda) & \text{(Bosons)} \\ 1-f(\epsilon_\lambda) & \text{(Fermions)}\end{array}\right. \tag{9.18}$$

Using the time evolution of the operators,

$$\begin{aligned} \psi_\lambda(\tau) &= e^{-\epsilon_\lambda \tau}\psi_\lambda(0) \\ \psi^\dagger{}_\lambda(\tau) &= e^{\epsilon_\lambda\tau}\psi^\dagger{}_\lambda(0)\end{aligned} \tag{9.19}$$

we deduce that

$$\mathcal{G}_{\lambda\lambda'}(\tau-\tau') = -\Big[\theta(\tau-\tau')\langle\psi_\lambda\psi^\dagger{}_{\lambda'}\rangle + \zeta\theta(\tau'-\tau)\langle\psi^\dagger{}_{\lambda'}\psi_\lambda\rangle\Big]e^{-\epsilon_\lambda(\tau-\tau')} \tag{9.20}$$

where we have re-introduced $\zeta = 1$ for Bosons and -1 for fermions, from Chapter 8. If we now write $\mathcal{G}_{\lambda\lambda'}(\tau-\tau') = \delta_{\lambda\lambda'}\mathcal{G}_\lambda(\tau-\tau')$, then

$$\mathcal{G}_\lambda(\tau) = -e^{-\epsilon_\lambda\tau}.\left\{\begin{array}{ll} [(1+n(\epsilon_\lambda))\theta(\tau) + n(\epsilon_\lambda)\theta(-\tau)] & \text{(Bosons)} \\ [(1-f(\epsilon_\lambda))\theta(\tau) - f(\epsilon_\lambda)\theta(-\tau)] & \text{(Fermions)}\end{array}\right. \tag{9.21}$$

There are several points to notice about this Green's function:

- Apart from prefactors, at zero temperature the imaginary time Green's function $\mathcal{G}_\lambda(\tau)$ is equal to zero-temperature Green's function $G_\lambda(t)$, evaluated at a time $t = -i\tau$, $\mathcal{G}_\lambda(\tau) = -iG_\lambda(-i\tau)$.
- If $\tau < 0$ the Green function satisfies the relation

  $$\mathcal{G}_{\lambda\lambda'}(\tau+\beta) = \zeta\mathcal{G}_{\lambda\lambda'}(\tau)$$

  so that the bosonic Green function is periodic in imaginary time, while the fermionic Green function is antiperiodic in imaginary time, with period β.

9.2.1 Periodicity and Antiperiodicity

The (anti) periodicity observed in the last example is actually a general property of finite temperature Green functions. To see this, take $-\beta < \tau < 0$, then we can expand the Green function as follows

$$\begin{aligned} \mathcal{G}_{\lambda\lambda'}(\tau) &= \zeta\langle\psi^\dagger{}_{\lambda'}(0)\psi_\lambda(\tau)\rangle \\ &= \zeta\mathrm{Tr}\left[e^{-\beta(H-F)}\psi^\dagger{}_{\lambda'}e^{\tau H}\psi_\lambda e^{-\tau H}\right]\end{aligned} \tag{9.22}$$

Now we can use the periodicity of the trace $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$ to cycle the operators on the left of the trace over to the right of the trace, as follows

$$\begin{aligned} \mathcal{G}_{\lambda\lambda'}(\tau) &= \zeta\mathrm{Tr}\left[e^{\tau H}\psi_\lambda e^{-\tau H}e^{-\beta(H-F)}\psi^\dagger{}_{\lambda'}\right] \\ &= \zeta\mathrm{Tr}\left[e^{\beta F}e^{\tau H}\psi_\lambda e^{-(\tau+\beta)H}\psi^\dagger{}_{\lambda'}\right] \\ &= \zeta\mathrm{Tr}\left[e^{-\beta(H-F)}e^{(\tau+\beta)H}\psi_\lambda e^{-(\tau+\beta)H}\psi^\dagger{}_{\lambda'}\right] \\ &= \zeta\mathrm{Tr}\langle\psi_\lambda(\tau+\beta)\psi^\dagger{}_{\lambda'}(0)\rangle \\ &= \zeta\mathcal{G}_{\lambda\lambda'}(\tau+\beta)\end{aligned} \tag{9.23}$$

This periodicity, or antiperiodicity was noted by Matsubara[1]. In the late 1950's, Abrikosov, Gorkov and Dzyalozinski[2] observed that we are in fact at liberty to extend the function outside $G(\tau)$ outside the range $\tau \in [-\beta,\beta]$ by assuming that this periodicity, or antiperiodicity extends indefinitely along the entire imaginary time axis. In otherwords, there need be no constraint on the value of τ in the periodic or antiperiodic boundary conditions

$$\mathcal{G}_{\lambda\lambda'}(\tau+\beta) = \pm\mathcal{G}_{\lambda\lambda'}(\tau)$$

With this observation, it becomes possible to carry out a Fourier expansion of the Green function in terms of discrete, frequencies. Today we use the term coined by Abrikosov, Gorkov and Dzyaloshinskii, calling them "Matsubara" frequencies[2].

9.2.2 Matsubara Representation

The Matsubara frequencies are defined as

$$\begin{aligned} \nu_n &= 2\pi n k_B T \qquad \text{(Boson)} \\ \omega_n &= \pi(2n+1)k_B T \qquad \text{(Fermion).}\end{aligned} \tag{9.24}$$

where by convention, ν_n is reserved for Bosons and ω_n for fermions. These frequencies have the property that

$$\begin{aligned} e^{i\nu_n(\tau+\beta)} &= e^{i\nu_n\tau} \\ e^{i\omega_n(\tau+\beta)} &= -e^{i\omega_n\tau}\end{aligned} \tag{9.25}$$

The periodicity or antiperiodicity of the Green function is then captured by expanding it as a linear sum of these functions:

$$\mathcal{G}_{\lambda\lambda'}(\tau) = \left\{\begin{array}{ll} T\sum_n \mathcal{G}_{\lambda\lambda'}(i\nu_n)e^{-i\nu_n\tau} & \text{Boson} \\ T\sum_n \mathcal{G}_{\lambda\lambda'}(i\omega_n)e^{-i\omega_n\tau} & \text{Fermion}\end{array}\right. \tag{9.26}$$

and the inverse of these relations is given by

$$\mathcal{G}_{\lambda\lambda'}(i\alpha_n) = \int_0^\beta d\tau \mathcal{G}_{\lambda\lambda'}(\tau) e^{i\alpha_n\tau}, \qquad (\alpha_n = \{\text{Matsubara frequency}\}) \tag{9.27}$$

Example : Free Fermions and Free Bosons

For example, let us use (9.27) to derive the propagator for non-interacting fermions or bosons with $H = \sum \epsilon_\lambda \psi^\dagger{}_\lambda \psi_\lambda$. For fermions, the Matsubara frequencies are $i\omega_n = \pi(2n+1)k_BT$ so using the real time propagator(9.21), we obtain

$$\begin{aligned} \mathcal{G}_\lambda(i\omega_n) &= -\int_0^\beta d\tau e^{(i\omega_n - \epsilon_\lambda)\tau} \overbrace{(1 - f(\epsilon_\lambda))}^{[1+e^{-\beta\epsilon_\lambda}]^{-1}} \\ &= -\frac{1}{i\omega_n - \epsilon_\lambda} \frac{\overbrace{(e^{(i\omega_n - \epsilon_\lambda)} - 1)}^{-1}}{1 + e^{-\beta\epsilon_\lambda}} \end{aligned} \tag{9.28}$$

so that

$$\boxed{\mathcal{G}_\lambda(i\omega_n) = \frac{1}{i\omega_n - \epsilon_\lambda} \qquad \textbf{Free Fermions}} \tag{9.29}$$

In a similar way, for free Bosons, where the Matsubara frequencies are $i\nu_n = \pi 2nk_BT$, using (9.27) and (9.21), we obtain

$$\begin{aligned} \mathcal{G}_\lambda(i\nu_n) &= -\int_0^\beta d\tau e^{(i\nu_n - \epsilon_\lambda)\tau} \overbrace{(1 + n(\epsilon_\lambda))}^{[1-e^{-\beta\epsilon_\lambda}]^{-1}} \\ &= -\frac{1}{i\nu_n - \epsilon_\lambda} \frac{\overbrace{(e^{(i\nu_n - \epsilon_\lambda)} - 1)}^{-1}}{1 - e^{-\beta\epsilon_\lambda}} \end{aligned} \tag{9.30}$$

so that

$$\boxed{\mathcal{G}_\lambda(i\nu_n) = \frac{1}{i\nu_n - \epsilon_\lambda} \qquad \textbf{Free Bosons}} \tag{9.31}$$

Remarks

- Notice how the finite temperature propagators (9.29) and (9.31) are essentially identical for free fermions and bosons. All the information about the statistics is encoded in the Matsubara frequencies.

- With the replacement $\omega \to i\omega_n$ the finite temperature propagator for Free fermions (9.29) is essentially identical to the zero temperature propagator, but notice that the inconvenient $i\delta\text{sign}(\epsilon_\lambda)$ in the denominator has now disappeared.

Example: Finite temperature Propagator for the Harmonic Oscillator

As a second example, let us calculate the finite temperature Green function

$$D(\tau) = -\langle T x(\tau) x(0)\rangle \tag{9.32}$$

and its corresponding propagator

$$D(i\nu) = \int_0^\beta e^{i\nu_n\tau} D(\tau) \tag{9.33}$$

for the simple harmonic oscillator

$$\begin{aligned} H &= \hbar\omega(b^\dagger b + \frac{1}{2}) \\ x &= \sqrt{\frac{\hbar}{2m\omega}}(b + b^\dagger) \end{aligned} \tag{9.34}$$

Expanding the Green function in terms of the creation and annihilation operators, we have

$$\begin{aligned} D(\tau) &= -\frac{\hbar}{2m\omega}\langle T(b(\tau) + b^\dagger(\tau))(b(0) + b^\dagger(0))\rangle \\ &= -\frac{\hbar}{2m\omega}\Big(\langle Tb(\tau)b^\dagger(0)\rangle + \langle Tb^\dagger(\tau)b(0)\rangle\Big), \end{aligned} \tag{9.35}$$

where terms involving two creation or two annihilation operators vanish. Now using the derivations that led to (9.21)

$$-\langle Tb(\tau)b^\dagger(0)\rangle = \mathcal{G}(\tau) = -[(1 + n(\omega))\theta(\tau) + n(\omega)\theta(-\tau)]e^{-\omega\tau}. \tag{9.36}$$

and

$$\begin{aligned} -\langle Tb^\dagger(\tau)b(0)\rangle &= -[n(\omega)\theta(\tau) + (1 + n(\omega))]e^{\omega\tau} \\ &= [(1 + n(-\omega))\theta(\tau) + n(-\omega)\theta(-\tau)]e^{\omega\tau}. \end{aligned} \tag{9.37}$$

which corresponds to $-\mathcal{G}(\tau)$ with the sign of ω inverted. With this observation,

$$D(\tau) = \frac{\hbar}{2m\omega}\left[G(\tau) - \{\omega \to -\omega\}\right]. \tag{9.38}$$

When we Fourier transform the first term inside the brackets, we obtain $\frac{1}{i\nu_n - \omega}$, so that

$$\begin{aligned} D(i\nu_n) &= \frac{\hbar}{2m\omega}\left[\frac{1}{i\nu_n - \omega} - \frac{1}{i\nu_n + \omega}\right] \\ &= \frac{\hbar}{2m\omega}\left[\frac{2\omega}{(i\nu_n)^2 - \omega^2}\right]. \end{aligned} \tag{9.39}$$

This expression is identical to the corresponding zero temperature propagator, evaluated at frequency $z = i\nu_n$.

Example 9.1: Consider a system of non-interacting Fermions, described by the Hamiltonian $H = \sum_\lambda \epsilon_\lambda c^\dagger{}_\lambda c_\lambda$ where $\epsilon_\lambda = E_\lambda - \mu$ and E_λ is the energy of a one-particle eigenstate and μ is the chemical potential.

Show that the total number of particles in equilibrium is

$$N(\mu) = T\sum \mathcal{G}_\lambda(i\omega_n)e^{i\omega_n 0^+}$$

where $\mathcal{G}_\lambda(i\omega_n) = (i\omega_n - \epsilon_\lambda)^{-1}$ is the Matsubara propagator. Using the relationship $N = -\partial F/\partial\mu$ show that that Free energy is given by

$$F(T,\mu) = -k_B T\sum_{\lambda,i\omega_n} \ln\left[-\mathcal{G}_\lambda(i\omega_n)^{-1}\right]e^{i\omega_n 0^+} + C(T) \tag{9.40}$$

Solution: The number of particles in state λ can be related to the equal time Green's function as follows

$$N_\lambda = \langle c^\dagger{}_\lambda c_\lambda\rangle = -\langle T c_\lambda(0^-)c^\dagger{}_\lambda\rangle = \mathcal{G}_\lambda(0^-).$$

Rewriting $G_\lambda(\tau) = T\sum_{i\omega_n}\mathcal{G}_\lambda e^{-i\omega_n\tau}$, we obtain

$$N(\mu) = \sum_\lambda N_\lambda = T\sum_{\lambda,i\omega_n}\mathcal{G}_\lambda(i\omega_n)e^{i\omega_n 0^+}$$

Now since $-\partial F/\partial\mu = N(\mu)$, it follows that

$$\begin{aligned} F &= -\int^\mu d\mu N(\mu) = -T\sum_{\lambda,i\omega_n}\int^\mu d\mu\frac{e^{i\omega_n 0^+}}{i\omega_n - E_\lambda + \mu} \\ &= -T\sum_{\lambda,i\omega_n}\ln\left[\epsilon_\lambda - i\omega_n\right]e^{i\omega_n 0^+} \\ &= -T\sum_{\lambda,i\omega_n}\ln\left[-\mathcal{G}_\lambda(i\omega_n)^{-1}\right]e^{i\omega_n 0^+} + C(T). \end{aligned} \tag{9.41}$$

We shall shortly see that $C = 0$ using Contour integral methods.

Example 9.2: Consider an electron gas where the spins are coupled to a magnetic field, so that $\epsilon_\lambda \equiv \epsilon_{\mathbf{k}} - \mu_B\sigma B$. Write down an expression for the magnetization and by differentiating w.r.t the field B, show that the temperature dependent magnetic susceptibility is given by

$$\chi(T) = \left.\frac{\partial M}{\partial B}\right|_{B=0} = -2\mu_B^2 k_B T\sum_{\mathbf{k},i\omega_n} G(k)^2$$

where $\mathcal{G}(k) \equiv G(\mathbf{k}, i\omega_n)$ is the Matsubara propagator.

Solution: The magnetization is given by

$$M = \mu_B\sum_{\lambda,\sigma}\sigma\langle c^\dagger{}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle = \mu_B T\sum_{\mathbf{k}\sigma,i\omega_n}\sigma\mathcal{G}_\sigma(\mathbf{k},i\omega_n)e^{i\omega_n 0^+}$$

Differentiating this w.r.t. B and then setting $B = 0$, we obtain

$$\begin{aligned} \chi &= \left.\frac{\partial M}{\partial B}\right|_{B=0} = -\mu_B^2 T\sum_{\mathbf{k}\sigma i\omega_n}\sigma^2\mathcal{G}_\sigma(\mathbf{k},i\omega_n)^2\Big|_{B=0} \\ &= -2\mu_B^2 k_B T\sum_{\mathbf{k},i\omega_n} G(k)^2 \end{aligned} \tag{9.42}$$

9.3 The contour integral method

In practice, we shall do almost all of our finite temperature calculations in the frequency domain. To obtain practical results, we will need to be able to sum over the Matsubara frequencies, and this forces us to make an important technical digression. As an example of the kind of tasks we might want to carry out, consider how we would calculate the occupancy of a given momentum state in a Fermi gas at finite temperature, using the Matsubara propagator $G(\mathbf{p}, i\omega_n)$. This can be written in terms of the equal time Green function, as follows

$$\langle c^\dagger{}_{\mathbf{p}\sigma}c_{\mathbf{p}\sigma}\rangle = \mathcal{G}(\mathbf{p},0^-) = T\sum_n\frac{1}{i\omega_n - \epsilon(\mathbf{p})}e^{i\omega_n 0^+}. \tag{9.43}$$

A more involved example, is the calculation of the finite temperature dynamical spin susceptibility $\chi(q)$ of the Free electron gas at wavevector and frequency $q \equiv (\mathbf{q}, i\nu_n)$. We shall see that this quantity derives from a Feynman polarization bubble diagram which gives

$$\chi(q) = -2\mu_B^2 T\sum_p \mathcal{G}(p+q)\mathcal{G}(p) = 2\mu_B^2\sum_{\mathbf{p}}\left(k_B T\sum_r G(\mathbf{p}+\mathbf{q}, i\omega_r + i\nu_n)G(\mathbf{p}, i\omega_r)\right). \tag{9.44}$$

where the -1 derives from the Fermion loop. In both cases, we need to know how to do the sum over the discrete Matsubara frequencies, and to do this, we use the method of contour integration. To make this possible, observe that the Fermi function $f(z) = 1/[e^{z\beta}+1]$ has poles of strength $-k_B T$ at each discrete frequency $z = i\omega_n$, because

$$f(i\omega_n + \delta) = \frac{1}{e^{\beta(i\omega_n+\delta)}+1} = -\frac{1}{\beta\delta} = -\frac{k_B T}{\delta}$$

so that for a general function $F(i\omega_n)$, we may write

$$k_B T\sum_n F(i\omega_n) = -\int_C\frac{dz}{2\pi i}F(z)f(z) \tag{9.45}$$

where the contour integral C is to be taken anticlockwise around the poles at $z = i\omega_n$ as shown in Fig. 9.3 (a)

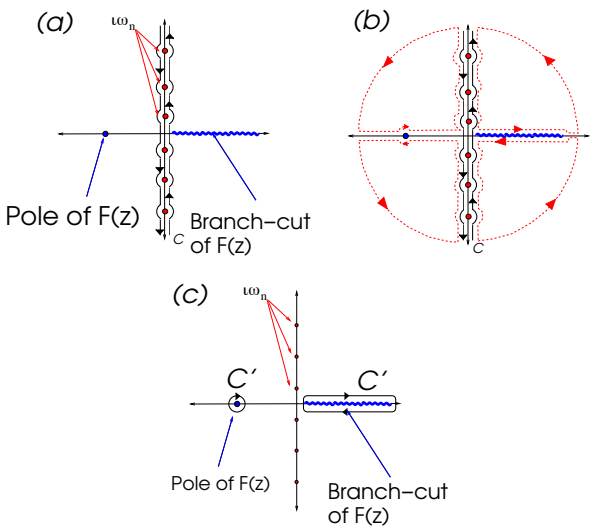


Figure 9.3: (a) Contour integration around the poles in the Fermi function enables us to convert a discrete Matsubara sum $T\sum F(i\omega_n)$ to a continuous integral (b) The integral can be distorted around the poles and branch-cuts of $F(z)$ provided that $F(z)$ dies away faster than $1/|z|$ at infinity.

Once we have cast the sum as a contour integral, we may introduce "null" contours (Fig. 9.3 (b)) which allow us to distort the original contour C into the modified contour C' shown in Fig. 9.3 (c), so that now

$$k_BT\sum_n F(i\omega_n) = -\int_{C'}\frac{dz}{2\pi i}F(z)f(z) \tag{9.46}$$

where C' runs *clockwise* around all the poles and branch-cuts in $F(z)$. Here we have used "Jordan's lemma" which guarantees that the contribution to the integral from the contour at infinity vanishes, provided the function $F(z)\times f(z)$ dies away faster than $1/|z|$ over the whole contour.

For example, in case (9.43), $F(z) = \frac{e^{z0^+}}{z-\epsilon_{\mathbf{p}}}$, so that $F(z)$ has a single pole at $z=\epsilon_{\mathbf{p}}$, and hence

$$\begin{aligned}\langle n_{\mathbf{p}\sigma}\rangle &= T\sum_n \frac{1}{i\omega_n-\epsilon(\mathbf{p})}e^{i\omega_n O^+} = -\int_{C'}\frac{dz}{2\pi i}\frac{1}{z-\epsilon_{\mathbf{p}}}e^{z0^+}f(z)\\ &= f(\epsilon_{\mathbf{p}}),\end{aligned} \tag{9.47}$$

recovering the expected result. In this example, the convergence factor e^{z0^+} that results from the small negative time increment in the Green function, plays an important role inside the Contour integral, where it gently forces the function $F(z)$ to die away faster than $1/|z|$ in the negative half-plane. Of course the original contour C integral could have been made by arbitrarily replacing $f(z)$ with $f(z)-$constant. However, the requirement that the function dies away in the positive half plane forces us to set the constant term here to zero.

In the second example (9.44)

$$F(z) = G(\mathbf{p}+\mathbf{q}, i\nu_n+z)G(\mathbf{p},z) = \frac{1}{i\nu_n+z-\epsilon_{\mathbf{p}+\mathbf{q}}}\frac{1}{z-\epsilon_{\mathbf{p}}}$$

which has two poles at $z=\epsilon_{\mathbf{p}}$ and $z=-i\nu_n+\epsilon_{\mathbf{p}+\mathbf{q}}$. The integral for this case is then given by

$$\begin{aligned}\chi(q) &= 2\mu_B^2\sum_{\mathbf{p}}\int_{C'}\frac{dz}{2\pi i}G(\mathbf{p}+\mathbf{q},z+i\nu_n)G(\mathbf{p},z)f(z)\\ &= -\sum_{\mathbf{p}}\Big(G(\mathbf{p},-i\nu_n+\epsilon_{\mathbf{p}+\mathbf{q}})f(-i\nu_n+\epsilon_{\mathbf{p}+\mathbf{q}}) + G(\mathbf{p}+\mathbf{q},\epsilon_{\mathbf{p}})f(\epsilon_{\mathbf{p}})\Big)\end{aligned} \tag{9.48}$$

The first term in the above expression deserves some special attention. In this term we shall make use the periodicity of the Fermi function to replace

$$f(-i\nu_n+\epsilon_{\mathbf{p}+\mathbf{q}}) = f(\epsilon_{\mathbf{p}+\mathbf{q}}).$$

This replacement may seem obvious, however, later, when analytically extending $i\nu_n\to z$ we will keep this quantity *fixed*, i.e, we will not analytically extend $f(-i\nu_n+\epsilon_{\mathbf{p}+\mathbf{q}})\to f(-z+\epsilon_{\mathbf{p}+\mathbf{q}})$. In other words, the Matsubara sum and the replacement $i\nu_n\to z$ are not to be commuted. With this understanding, we continue, and find that the resulting expression is given by

$$\chi(\mathbf{q},i\nu_n) = 2\mu_B^2\sum_{\mathbf{p}}\left(\frac{f_{\mathbf{p}+\mathbf{q}}-f_{\mathbf{p}}}{i\nu_n-(\epsilon_{\mathbf{p}+\mathbf{q}}-\epsilon_{\mathbf{p}})}\right) \tag{9.49}$$

where we have used the shorthand $f_{\mathbf{p}}\equiv f(\epsilon_{\mathbf{p}})$. The analytic extension of this quantity is then

$$\chi(\mathbf{q},z) = 2\mu_B^2\sum_{\mathbf{p}}\left(\frac{f_{\mathbf{p}+\mathbf{q}}-f_{\mathbf{p}}}{z-(\epsilon_{\mathbf{p}+\mathbf{q}}-\epsilon_{\mathbf{p}})}\right) \tag{9.50}$$

A completely parallel set of procedures can be carried for summation over Matsubara boson frequencies $i\nu_n$, by making the observation that the Bose function $n(z)=\frac{1}{e^{\beta z}-1}$ has a string of poles at $z=i\nu_n$ of strength k_BT. Using a completely parallel procedure to the fermions, we obtain

$$k_BT\sum_n P(i\nu_n) = \int_C\frac{dz}{2\pi i}P(z)n(z) = \int_{C'}\frac{dz}{2\pi i}P(z)n(z)$$

where C is an anticlockwise integral around the imaginary axis and C' is a clockwise integral around the poles and branch-cuts of $F(z)$. (See problem 9.1.)

Example 9.3: Starting with the expression

$$F = -T\sum_{\lambda i\omega_n} \ln[(\epsilon_\lambda - i\omega_n)]e^{i\omega_n 0^+} + C(T)$$

derived in example (9.1), use the contour integration method to show that

$$F = -T\sum_{\lambda} \ln\left[1 + e^{-\beta\epsilon_\lambda}\right] + C(T)$$

so that $C(T) = 0$.

Solution: Writing the Free energy as a contour integral around the poles of the imaginary axis, we have

$$F = \sum_\lambda \int_P \frac{dz}{2\pi i} f(z) \ln\left[\epsilon_\lambda - z\right] e^{z0^+} + C(T)$$

where the path P runs anticlockwise around the imaginary axis. There is a branch cut in the function $F(z) = \ln[\epsilon_\lambda - z]$ running from $z = \epsilon_\lambda$ to $z = +\infty$. If we distort the contour P around this branch-cut, we obtain

$$F = \sum_\lambda \int_{P'} \frac{dz}{2\pi i} f(z) \ln\left[\epsilon_\lambda - z\right] e^{z0^+} + C(T)$$

where P' runs clockwise around the branch cut, so that

$$\begin{aligned} F &= \sum_\lambda \int_{\epsilon_\lambda}^{\infty} \frac{d\omega}{\pi} f(\omega) + C(T) \\ &= \sum_\lambda -T\ln(1 + e^{-\beta\epsilon_\lambda}) + C(T) \end{aligned} \tag{9.51}$$

so that $C(T) = 0$, to reproduce the standard expression for the Free energy of a set of non-interacting fermions.

9.4 Generating Function and Wick's theorem

The zero temperature generating functions for Free fermions or bosons, derived in chapter 7. can be generalized to finite temperatures. Quite generally we can consider adding a source term to a free particle Hamiltonian to form $H(\tau) = H_0 + V(\tau)$,

$$\left.\begin{aligned} H_0 &= \textstyle\sum \epsilon \psi^\dagger{}_\lambda \psi_\lambda \\ V(\tau) &= -\textstyle\sum_\lambda [\bar\eta_\lambda(\tau)\psi_\lambda + \psi^\dagger{}_\lambda \eta(\tau)] \end{aligned}\right\} \tag{9.52}$$

The corresponding finite temperature Generating functional is actually the partition function in the presence of the perturbation V. Using a simple generalization of (9.13), we have

$$\begin{aligned} Z_0[\bar\eta,\eta] &= Z_0\langle T e^{-\int_0^\beta V_I(\tau)d\tau}\rangle_0 \\ &= Z_0\langle T\exp\left[\int_0^\beta d\tau \sum_\lambda \left(\bar\eta_\lambda(\tau)\psi_\lambda(\tau) + \psi^\dagger{}_\lambda(\tau)\eta_\lambda(\tau)\right)\right]\rangle_0 \end{aligned} \tag{9.53}$$

where the driving terms are complex numbers for bosons, but are anticommuting C-numbers or Grassman numbers, for fermions. For free fields, the Generating functional is given by

$$\boxed{\begin{aligned} \frac{Z_0[\bar\eta,\eta]}{Z_0} &= \exp\left[-\sum_\lambda \int_0^\beta d\tau_1 d\tau_2 \bar\eta_\lambda(1) G_\lambda(\tau_1 - \tau_2)\eta_\lambda(2)\right] \\ G_\lambda(\tau_1 - \tau_2) &= -\langle T\psi_\lambda(\tau_1)\psi^\dagger{}_\lambda(\tau_2)\rangle \end{aligned}} \tag{9.54}$$

A detailed proof of this result is given in Appendix A of this chapter. However, a heuristic proof is obtained by appealing to the "Gaussian" nature of the underlying Free fields. As at zero temperature, we expect the the physics to be entirely Gaussian, that is, that the amplitudes of fluctuation of the free fields are entirely independent of the driving terms. The usefulness of the generating function, is that we can convert partial derivatives with respect to the source terms into field operators inside the expectation values,

$$\begin{aligned} \frac{\delta}{\delta\bar\eta(1)} &\rightarrow \psi^\dagger(1), \\ \frac{\delta}{\delta\eta(2)} &\rightarrow \zeta\psi^\dagger(2), \end{aligned} \tag{9.55}$$

where we have used the short-hand notation $\eta(1) \equiv \eta_\lambda(\tau_1), \psi(1) \equiv \psi_\lambda(\tau_1))$. In particular

$$\frac{\delta \ln Z_0[\bar\eta,\eta]}{\delta\bar\eta(2)} = \langle\psi(2)\rangle, \tag{9.56}$$

where the derivative of the logarithm of $Z_0[\bar\eta,\eta]$ is required to place a $Z_0[\bar\eta,\eta]$ in the denominator for the correctly normalized expectation value. For bosons, you can think of the source terms as an external field that induces a condensate of the field operator. At high temperatures, once the external source term is removed, the condensate disappears. However, at low temperatures, in a Bose-Einstein condensate, the expectation value of the field survives even when the source terms are removed. For fermions, the idea of a genuine expectation value for the Fermi field is rather abstract, and in this case, once the external source is removed, the expectation value disappears.

We can of course take higher derivatives, and these do not vanish, even when the source terms are removed. In particular the second derivative determines the fluctuations of the quantum field, given by

$$\frac{\delta^2 \ln Z_0[\bar\eta,\eta]}{\delta\eta(1)\delta\bar\eta(2)} = \frac{\delta}{\delta\eta(1)}\left[\frac{1}{Z_0[\bar\eta,\eta]}\frac{\delta Z_0[\bar\eta,\eta]}{\delta\bar\eta(2)}\right]$$

$$
\begin{aligned}
&= \frac{1}{Z_0[\bar\eta,\eta]}\frac{\delta^2 Z_0[\bar\eta,\eta]}{\delta\eta(1)\delta\bar\eta(2)} - \frac{1}{Z_0[\bar\eta,\eta]}\left[\frac{\delta Z_0[\bar\eta,\eta]}{\delta\eta(1)}\right]\frac{1}{Z_0[\bar\eta,\eta]}\left[\frac{\delta Z_0[\bar\eta,\eta]}{\delta\bar\eta(2)}\right]\\
&= \zeta\Big(\langle T\psi^\dagger(2)\psi(1)\rangle - \langle\psi^\dagger(2)\rangle\langle\psi(1)\rangle\Big)\\
&= \langle T\psi(1)\psi^\dagger(2)\rangle - \langle\psi(1)\rangle\langle\psi^\dagger(2)\rangle\\
&= \langle T\Big(\psi(1)-\langle\psi(1)\rangle\Big)\Big(\psi^\dagger(2)-\langle\psi^\dagger(2)\rangle\Big)\rangle = \langle\delta\psi(1)\delta\psi^\dagger(2)\rangle, \qquad (9.57)
\end{aligned}
$$

where $\delta\psi(1) = \psi(1) - \langle\psi(1)\rangle$ represents the fluctuation of the field ψ around its mean value. If this quantity is independent of the source terms, then it follows that the fluctuations must be equal to their value in the absence of any source field, i.e.

$$
\frac{\delta^2 \ln Z_0[\bar\eta,\eta]}{\delta\bar\eta_\lambda(\tau_1)\delta\eta_\lambda(\tau_2)} = \frac{\delta^2 \ln Z_0[\bar\eta,\eta]}{\delta\bar\eta_\lambda(\tau_1)\delta\eta_\lambda(\tau_2)}\bigg|_{\eta=\bar\eta=0} = -\mathcal{G}_\lambda(\tau_1-\tau_2).
$$

A more detailed, algebraic rederivation of this result is given in Appendix A. One of the immediate corolloraries of (9.128) is that the multi-particle Green functions can be entirely decomposed in terms of one-particle Green functions, i.e., the imaginary time Green functions obey a Wick's theorem. If we decompose the original generating function (9.127) into a power series, we find that the general coefficient of the source terms is given by

$$
(-1)^n\mathcal{G}(1,2,\ldots n;1',2',\ldots n') = \langle T\psi(1)\ldots\psi(n)\psi^\dagger(n')\ldots\psi(1')\rangle
$$

by contrast, if we expand the right-hand side of (9.128) in the same way, we find that the same coefficient is given by

$$
(-1)^n\sum_P(\zeta)^p\prod_{r=1}^n\mathcal{G}(r-P_r)
$$

where p is the number of pairwise permutations required to produce the permutation P. Comparing the two results, we obtain the imaginary time Wick's theorem

$$
\boxed{\mathcal{G}(1,2,\ldots n;1',2',\ldots n') = \sum_P(-1)^p\prod_{r=1}^n\mathcal{G}(r-P_r)}
$$

Although this result is the precise analog of the zero-temperature Wick's theorem, notice that that unlike its zero-temperature counterpart, we can not easily derive this result for simple cases by commuting the destruction operators so that they annihilate against the vacuum, since there is no finite temperature vacuum.

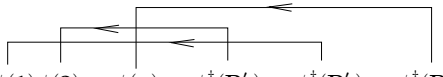
Just as in the zero temperature case, we can define a "contraction" as the process of connecting

two free -field operators inside the correlation function,

$$
\langle T[\ldots\psi(\mathbf{1})\ldots\psi^\dagger(\mathbf{2})\ldots]\rangle \longrightarrow \langle T[\psi(\mathbf{1})\psi^\dagger(\mathbf{2})]\rangle = -G(\mathbf{1}-\mathbf{2})
$$

$$
\langle T[\ldots\psi^\dagger(\mathbf{2})\ldots\psi(\mathbf{1})\ldots]\rangle \longrightarrow \langle T[\psi^\dagger(\mathbf{2})\psi(\mathbf{1})]\rangle = -\zeta G(\mathbf{1}-\mathbf{2})
$$

so that as before,



$$
\begin{aligned}
&(-1)^n\langle T[\psi(\mathbf{1})\psi(\mathbf{2})\ldots\psi(\mathbf{n})\ldots\psi^\dagger(\mathbf{P'_2})\ldots\psi^\dagger(\mathbf{P'_1})\ldots\psi^\dagger(\mathbf{P'_n})]\rangle\\
&= \zeta^P G(\mathbf{1}-P'_1)G(\mathbf{2}-P'_2)\ldots G(\mathbf{n}-P'_n). \qquad (9.58)
\end{aligned}
$$

Example 9.4:

Use Wick's theorem to calculate the interaction energy of a dilute Bose gas of spin S bosons particles interacting via a the interaction

$$
\hat V = \frac{1}{2}\sum_{q,k\sigma,k',\sigma'}V(q)b^\dagger{}_{k+q\sigma}b^\dagger{}_{k'\sigma'}b_{k'+q\sigma'}b_{k\sigma}
$$

at a temperature above the Bose Einstein condensation temperature.

Solution: To leading order in the interaction strength, the interaction energy is given by

$$
\langle V\rangle = \sum_{q,k,k',\sigma,\sigma'}V(q)\langle b^\dagger{}_{k+q,\sigma}b^\dagger{}_{k',\sigma'}b_{k'+q,\sigma'}b_{k\sigma}\rangle
$$

Using Wick's theorem, we evalute

$$
\begin{aligned}
\langle b^\dagger{}_{k+q,\sigma}b^\dagger{}_{k',\sigma'}b_{k'+q,\sigma'}b_{k,\sigma}\rangle &= \langle b^\dagger_{k+q,\sigma}b^\dagger_{k',\sigma'}b_{k'+q,\sigma'}b_{k,\sigma}\rangle + \langle b^\dagger_{k+q,\sigma}b^\dagger_{k',\sigma'}b_{k'+q,\sigma'}b_{k,\sigma}\rangle\\
&= n_k n_{k'}\delta_{q,0} + n_k n_{k+q}\delta_{k,k'}\delta_{\sigma\sigma'} \qquad (9.59)
\end{aligned}
$$

so that

$$
\langle\hat V\rangle = \frac{1}{2}\int_{\mathbf{k},\mathbf{k'}}n_k n_{k'}\left[(2S+1)^2V_{q=0} + (2S+1)V_{k-k'}\right]
$$

where $n_{\mathbf{k}} = \frac{1}{e^{\beta(\epsilon_{\mathbf{k}}-\mu)}-1}$.

9.5 Feynman diagram expansion

We are now ready to generalize the Feynman approach to finite temperatures. Apart from a very small change in nomenclature, almost everything we learnt for zero temperature in chapter 8 now generalizes to finite temperature. Whereas previously, we began with a Wick expansion of the S matrix, now we must carry out a Wick expansion of the partition function

$$Z = e^{-\beta F} = Z_0 \langle T \exp\left[-\int_0^\beta \hat{V}(\tau) d\tau\right]\rangle_0 =$$

All the combinatorics of this expansion are unchanged at finite temperatures.

Now we are at finite temperature, the Free energy $F = E - ST - \mu N$ replaces the energy. The main results of this procedure can almost entirely be guessed by analogy. In particular:

- The partition function

$$Z = Z_0 \sum \{\text{Unlinked Feynman diagrams }\}$$

- The change in the Free energy due to the perturbation V is given by

$$\Delta F = F - F_0 = -k_B T \ln\left[\frac{Z}{Z_0}\right] = -k_B T \sum \{\text{Linked Feynman diagrams}\}$$

This is the finite temperature version of the linked cluster theorem.

- Matsubara one-particle Green's functions

$$\mathcal{G}(1-2) = \sum \{\text{Two-legged Feynman diagrams}\}$$

, and the main changes are

(i) the replacement of a $-i \longrightarrow -1$ in the time-ordered exponential.

(ii) the finite range of integration in time

$$\int_{-\infty}^{\infty} dt \to \int_0^\beta d\tau$$

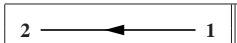
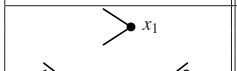
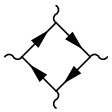
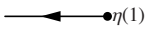
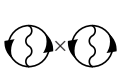
which leads to the discrete Matsubara frequencies.

The effect of these changes on the real-space Feynman rules is summarized in Table 9.1.

The book-keeping that leads to these diagrams now involves the redistribution of a "-1" associated with each propagator

$$\overbrace{\psi(2)\ldots\psi^\dagger(1)} \ \to (i)^2 \times \mathcal{G}(2-1). \tag{9.60}$$

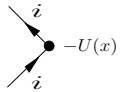
Table. 9.1 Real Space Feynman Rules: Finite Temperature .

	$G(\mathbf{2}-\mathbf{1})$
	$U(x_1)$ $-V(\mathbf{1}-\mathbf{2})$
$\prod_i \int d^3x_i \int_0^\beta d\tau$	Integrate over all intermediate times and positions.
 	$-(2S+1)G(\vec{0}, 0^-)$ $[-(2S+1)]^F$, F = no. Fermion loops.
	$\eta(1)$ $-\bar{\eta}(1)$
 $p = 2$  $p = 8$	$\frac{1}{p}$ p = order of symmetry group.

where as before,

$$\mathcal{G}(2-1) = 2 \longleftarrow 1 \tag{9.61}$$

represents the propagation of a particle from "1" to "2", but now we must redistribute an i (rather than a $\sqrt{-i}$) to each end of the progator. When these terms are redistributed onto one-particle scattering vertices, they cancel the -1 from the time-ordered exponential



$$-U(x) \qquad = (i)^2 \times -U(x) \equiv U(x) \tag{9.62}$$

whereas for a two-particle scattering potential $V(1-2)$, the four factors of i give a $(i)^4 = 1$, so that the two-particle scattering amplitude is $-V(1-2)$.

$$= (i)^4 \times -V(1-2) \equiv -V(1-2). \tag{9.63}$$

Apart from these small changes, the real-time Feynman rules are basically the same as those at zero temperature.

9.5.1 Feynman rules from Functional Derivatives

As in chapter 8, we can formally derive the Feynman rules from a functional derivative formulation. Using the notation

$$\int d1d2\bar{\eta}(1)\mathcal{G}(1-2)\eta(2) = \bar{\eta} \longleftarrow \eta \tag{9.64}$$

where $d1$ and $d2$ implies the integration over the space-time variables $(\vec{1}, \tau_1)$ and $(\vec{2}, \tau_2)$ and a sum over suppressed spin variables σ_1 and σ_2, we can write the non-interacting generating functional as

$$\frac{Z_0[\bar{\eta},\eta]}{Z_0} = \langle \hat{S} \rangle_0 = \exp\Big[-\bar{\eta} \longleftarrow \eta\Big] \tag{9.65}$$

where we have used the short-hand

$$\hat{S} = T\exp\left[\int_0^\beta d1[\bar{\eta}(1)\psi(1) + \psi^\dagger(1)\eta(1)]\right]$$

Now each time we differentiate $\hat{S}$ with respect to its source terms, we bring down an additional field operator, so that

$$\frac{\delta}{\delta\bar{\eta}(1)}\langle T\ldots\hat{S}\rangle_0 \;=\; \langle\ldots\psi(1)\ldots\hat{S}\rangle_0,$$

$$\frac{\delta}{\delta\eta(2)}\langle T\ldots\hat{S}\rangle_0 \;=\; \langle T\ldots\psi^\dagger(2)\ldots\hat{S}\rangle_0 \tag{9.66}$$

we can formally evaluate the time-ordered expectation value of any operator $F[\psi^\dagger,\psi]$ as

$$\langle TF\left[\psi^\dagger,\psi\right]\hat{S}\rangle_0 = F[\frac{\delta}{\delta\eta},\frac{\delta}{\delta\bar{\eta}}]\exp\Big[-\bar{\eta} \longleftarrow \eta\Big]$$

so that

$$\begin{aligned}\frac{Z[\bar{\eta},\eta]}{Z_0} &= \langle T exp\Big[-\int_0^\beta \hat{V}(\tau)d\tau\Big]\hat{S}\rangle_0 \\ &= \langle\exp\Big[-\int_0^\beta d\tau V\Big(\frac{\delta}{\delta\eta},\frac{\delta}{\delta\bar{\eta}}\Big)\Big]\exp\Big[-\bar{\eta} \longleftarrow \eta\Big]\end{aligned}$$

The formal expansion of this functional derivative generates the Feynman diagram expansion. Changing variables to $(\alpha,\bar{\alpha}) = (\eta,-\bar{\eta})$, we can remove the minus-sign associated with each propagator, to obtain

$$\frac{Z[-\bar{\alpha},\alpha]}{Z_0} = \exp\Big[(-1)^n\int_0^\beta d\tau V\Big(\frac{\delta}{\delta\alpha},\frac{\delta}{\delta\bar{\alpha}}\Big)\Big]\exp\Big[\bar{\alpha} \longleftarrow \alpha\Big] \tag{9.67}$$

for an $n-$ body interaction. The appearance of the $(-1)^n$ in the exponent indicates that we should associate a $(-1)^n$ with the corresponding scattering amplitude.

As in the case of zero temperature, we may regard (**??**) as a machine for generating a series of Feynman diagrams- both linked and unlinked, so that formally,

$$Z[\bar{\alpha},\alpha] = Z_0\sum\{\text{Unlinked Feynman diagrams}\}.$$

9.5.2 Feynman rules in frequency/momentum space

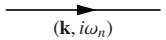
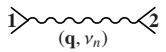
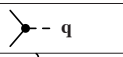
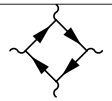
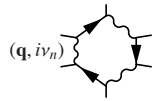
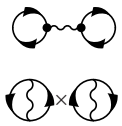
As at zero temperature, it is generally more convenient to work in Fourier space. The transformation to Fourier transform space follows precisely parallel lines to that at zero temperature, and the Feynman rules which result are summarized in Table 9.2. We first re-write each interaction line and Green's function in a Feynman diagram in terms of their Fourier transformed variables

$$\begin{aligned}1 \longrightarrow 2 \;&=\; G(X_1-X_2) = \sum_n\int\frac{d^{d-1}p}{(2\pi)^{d-1}}G(p)e^{ip(X_1-X_2)} \\ \text{1}\!\!\sim\!\!\text{2} \;&=\; V(X_1-X_2) = T\sum_n\int\frac{d^{d-1}q}{(2\pi)^{d-1}}V(q)e^{iq(X_1-X_2)}\end{aligned} \tag{9.68}$$

where we have used a short-hand notation $p = (\mathbf{p}, i\alpha_n)$ (where $\alpha_n = \omega_n$ for fermions, $\alpha_n = \nu_n$ for bosons), $q = (\mathbf{q}, i\nu_n)$, $X = (\mathbf{x}, i\tau)$, $ip.X = i\mathbf{p}\cdot\mathbf{x} - i\omega_n\tau$ and $iq.X = i\mathbf{q}\cdot\mathbf{x} - i\nu_r\tau$). As an example, consider a screened Coulomb interaction

$$V(r) = \frac{e^2}{r}e^{-\kappa r}$$

Table. 9.2 Momentum Space Feynman Rules: Finite Temperature .

 $(\mathbf{k}, i\omega_n)$	$G_o(\mathbf{k}, i\omega_n)$	Fermion propagator
 $(\mathbf{q}, \nu_n)$	$-V(q)$ $-g_q^2 D_o(\mathbf{q}, i\nu_n)$ $= -g_{\mathbf{q}}^2\left[\frac{2\omega_q}{(i\nu_n)^2 - \omega_{\mathbf{q}}^2}\right]$	Interaction Exchange Boson.
 q	$U(\mathbf{q})$	Scattering potential
	$[-(2S+1)]^F$,	F= no. Fermion loops
 $(\mathbf{q}, i\nu_n)$	$T\sum_n \int \frac{d^d q}{(2\pi)^d} e^{i\alpha_n 0^+}$	Sum over internal loop frequency and momenta.
 $p = 2$ $p = 8$	$\frac{1}{p}$	p = order of symmetry group.

In our space time notation, we write the interaction as

$$V(X) = V(\mathbf{x}, \tau) = \frac{e^2}{|\mathbf{x}|} e^{-\kappa|\mathbf{x}|} \times \bar{\delta}(\tau)$$

Where the delta function in time arises because the interaction is instantaneous. (Subtle point: we will in fact inforce periodic boundary conditions by taking the delta function to be a periodic delta function $\bar{\delta}(\tau) = \sum_n \delta(\tau - n\beta)$). When we Fourier transform this interaction, we obtain

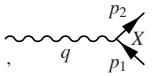
$$\begin{aligned} V(Q) = V(\mathbf{q}, i\nu_r) &= \int d^4X V(X) e^{-iQ.X} \\ &= \int d^3x \int_0^\beta d\tau V(\mathbf{x}) \bar{\delta}(\tau) e^{-i(\mathbf{q}\cdot\mathbf{x} - \nu_r \tau)} \\ &= V(\mathbf{q}) = \frac{4\pi e^2}{q^2 + \kappa^2} \end{aligned} \tag{9.69}$$

and the delta function in time translates to an interaction that is frequency independent.

We can also transform the source terms in a similar way, writing

$$\begin{aligned} \eta(X) &= T\sum_n \int \frac{d^{d-1}p}{(2\pi)^{d-1}} e^{ipX} \eta(p) \\ \bar{\eta}(X) &= T\sum_n \int \frac{d^{d-1}p}{(2\pi)^{d-1}} e^{-ipX} \bar{\eta}(p) \end{aligned} \tag{9.70}$$

where, $ipX = i\vec{p}\cdot\vec{x} - i\alpha_n\tau$. With these transformations, the space-time co-ordinates associated with each scattering vertex now only appear as "phase factors". By making the integral over space-time co-ordinates at each such vertex, we impose the conservation of momentum and (discrete) Matsubara frequencies at each vertex



$$= \int d^dX e^{i(p_1 - p_2 - q)X} = (2\pi)^3 \beta \delta^{(d-1)}(\mathbf{p}_1 - \mathbf{p}_2 - \mathbf{q}) \delta_{\alpha_1 + \alpha_2 - \nu_r} \tag{9.71}$$

Since momentum and frequency are conserved at each vertex, this means that there is one independent energy and frequency per loop in the Feynman diagram. To be sure that this really works, let us count the number of independent momenta that are left over after imposing a constraint at each vertex in the diagram. Consider a diagram with V vertices and P propagators. Each propagator introduces $P \times d$, momenta. When we integrate over the space-time co-ordinates of the V vertices, we must be careful to split the integral up into the integral over the $V - 1$ relative co-ordinates $\bar{X}_j = X_{j+1} - X_j$ and the center of mass co-ordinates:

$$\int \prod_{j=1}^{V} d^dX_j = \int d^dX_{CM} \int \prod_{j=1}^{V-1} d^d\bar{X}_j$$

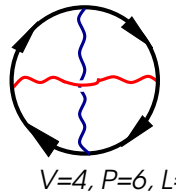
This imposes $(V - 1)$ constraints per dimension, so the number of independent momenta are then

$$\text{no. of independent momenta } = d[P - (V-1)]$$

Now in a general Feynman graph, the apparent number of momentum loops is the same as the number of facets in the graph, and this is given by

$$L = \mathcal{E} + (P - V)$$

where $\mathcal{E}$ is the Euler characteristic of the object. The Euler characteristic is equal to one for planar diagrams, and equal to one plus the number of "handles" in a non-planar diagram. For example, the diagram

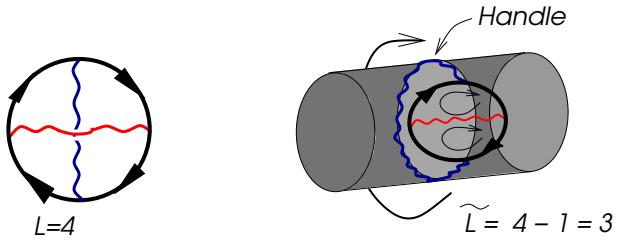


(9.72)

has $V = 4$ vertices, $P = 6$ propagators and it has one handle with Euler characteristic $E = 2$, so that $L = 6 - 4 + 2 = 4$ as expected. So from the above, we deduce that the number of independent momenta is given by

$$d[L - (E - 1)]$$

This result needs a moments pause. One might have expected number of independent momentum loops to be equal to L. However, when there are handles, this overcounts the number of independent momentum loops - for each handle added to the diagram adds only one additional momentum loop, but L increases by 2. If you look at our one example, this diagram can be embedded on a cylinder, and the interaction propagator which loops around the cylinder only counts as one momentum loop, giving a total of $4 - (2 - 1) = 3$ independent momentum loops.



(9.73)

In this way, we see that $\tilde{L} = L + (E - 1)$ *is* the correct number of independent momentum loops. Indeed, our momentum constraint does indeed convert the diagram from an integral over V space-time co-ordinates to $\tilde{L}$ independent momentum loops.

In this way, we see that the transformation from real-space, to momentum space Feynman rules is effected by replacing the sum over all internal space-time co-ordinates by an integral/sum over all loop momenta and frequencies. A convergence factor

$$e^{i\alpha_n 0^+}$$

is included in the loop integral. This term guarantees that if the loop contains a single propagator which propagates back to the point from which it eminated, then the corresponding contraction of field operators is normal ordered.

9.5.3 Linked Cluster Theorem

The linked cluster theorem for imaginary time follows from the replica trick, as at zero temperature. In this case, we wish to compute the logarithm of the partition function

$$ln(\frac{Z}{Z_0}) = \lim_{n\to 0} \frac{1}{n}\left[\left(\frac{Z}{Z_0}\right)^n - 1\right]$$

It is worth mentioning here that the replica trick was in fact originally invented by Edwards as a device for dealing with disorder- we shall have more to say about this in chapter 11.

We now write the term that contains $(Z/Z_0)^n$ as the product of contributions from n replica systems, so that

$$\left(\frac{Z}{Z_0}\right)^n = \left\langle \exp\left[-\int_0^\beta d\tau \sum_{\lambda=1}^{n} V^{(\lambda)}(\tau)\right]\right\rangle_0$$

When we expand the right-hand side as a sum over unlinked Feynman diagrams, each separate Feynman diagram has a replica index that must be summed over, so that a single linked diagram is of order $O(n)$, whereas a group of k unlinked diagrams is of order $O(n^k)$. In this way, as $n \to 0$, only the unlinked diagrams survive, so that. The upshot of this result is that the shift in the Free energy ΔF produced by the perturbation $\hat{V}$, is given by

$$-\beta\Delta F = \ln(Z/Z_0) = \sum\{\text{Closed link diagrams in real space}\}$$

Notice that unlike the zero temperature proof, here we do not have to appeal to adiabaticity to extract the shift in Free energy from the closed loop diagrams.

When we convert to momentum space, Fourier transforming each propagator and interaction line, an overall integral over the center of mass co-ordinates factors out of the entire diagram, giving rise to a prefactor

$$\int d^d X_{cm} = \beta(2\pi)^{d-1}\delta^{(d-1)}(0) \equiv V\beta$$

where V is the spatial volume. Consequently, expressed in momentum space, the change in Free energy is given by

$$\frac{\Delta F}{V} = -\sum\{\text{Closed linked diagrams in momentum space}\}.$$

Finally, let us say a few words about Green-functions Since the $n-th$ order coefficients of α and $\bar{\alpha}$ are the irreducible n-point Green-functions,

$$\begin{aligned}\ln Z[\bar{\alpha},\alpha] &= -\beta\Delta F + \int d1d2\bar{\alpha}(1)\mathcal{G}(1-2)\alpha(2) \\ &+ \frac{1}{(2!)^2}\int d1d2d3d4\bar{\alpha}(1)\bar{\alpha}(2)\alpha(3)\alpha(4)\mathcal{G}_{irr}(1,2;3,4)+\ldots. \end{aligned} \tag{9.74}$$

n-particle irreducible Green functions are simply the n-particle Green functions in which all contributions from $n-1$ particle Green functions have been subtracted. Now since the n-th order coefficients in the Feynman diagram expansion of $\ln Z[\bar{\alpha},\alpha]$ are the connected $2n$-point diagrams, it follows that the n-paricle irreducible Green functions are given by the sum of all $2n$ point diagrams

$$\mathcal{G}_{irr}(1,2,\ldots n;1',2',\ldots n') = \sum\{\text{Connected n-point diagrams}\}.$$

The main links between finite temperature Feynman diagrams and physical quantities are given in table 9.3.

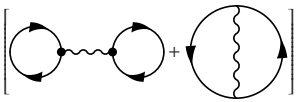
9.6 Examples of the application of the Matsubara Technique

To illustrate the Matsubara technique, we shall examine three examples. In the first, we will see briefly how the Hartree Fock approximation is modified at finite temperatures. This will give some familiarily with the techniques. In the second, we shall examine the effect of disorder on the electron propagator. Surprisingly, the spatial fluctuations in the electron potential that arise in a disordered medium behave like a highly retarded potential, and the scattering created by these fluctuations is responsible for the Drude lifetime in a disordered medium. As our third introductory example, we will examine an electron moving under the retarded interaction effects produced by the exchange of phonons, examining for the first time how inelastic scattering generates an electron lifetime.

9.6.1 Hartree Fock at a finite temperature.

As a first example, consider the Hartree-Fock correction to the Free energy,

$$\frac{\Delta F_{HF}}{V} = -\left[\quad\right] \tag{9.75}$$



These diagrams are precisely the same as those encountered in chapter 8, but now to evaluate them, we implement the finite temperature rules, which give,

$$\frac{\Delta F_{HF}}{V} = \frac{1}{2}\sum_k G(k)\sum_{k'}G(k')\left\{[-(2S+1)]^2 V(k-k') - (2S+1)V(q=0)\right\} \tag{9.76}$$

where the prefactor is the $p=2$ symmetry factor for these diagrams and

$$\sum_k G(k) \equiv \int_{\mathbf{k}} T\sum \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}} e^{i\omega_n 0^+}$$

Using the contour integration method introduced in section (9.3), following (9.47), we have

$$T\sum \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}} e^{i\omega_n 0^+} = \int_C \frac{dz}{2\pi i}\frac{1}{z-\epsilon_{\mathbf{k}}} e^{z0^+} f(z) = f(\epsilon_{\mathbf{k}}),$$

where the contour C runs anticlockwise around the pole at $z=\epsilon_{\mathbf{k}}$, so that the first order shift in the Free energy is

$$\Delta F_{HF} = \frac{1}{2}\int_{\mathbf{k},\mathbf{k}'}\left[(2S+1)^2(V_{\mathbf{q}=\mathbf{0}}) - (2S+1)(V_{\mathbf{k}-\mathbf{k}'})\right] f_{\mathbf{k}} f_{\mathbf{k}'}.$$

This is formally exactly the same as at zero temperature, excepting that now $f_{\mathbf{k}}$ refers to the finite temperature Fermi Dirac. Notice that we could have applied exactly the same method to bosons, the main result being a change in sign of the second Fock term.

9.6.2 Electron in a disordered potential

As a second example of the application of finite temperature methods, we shall consider the propagator for an electron in a disordered potential. This will introduce the concept of an "impurity average".

Our interest in this problem is driven ultimately by a desire to understand the bulk properties of a disordered metal. The problem of electron transport is almost as old as our knowledge of the electron itself. The term "electron" was first coined to describe the fundamental unit of charge (already measured from electrolysis) by the Irish physicist George Johnstone Stoney in 1891[3]. Heinrich Lorentz derived his famous force law for charged "ions" in 1895[4], but did not use the term electron until 1899. In 1897 J. J. ("JJ") Thomson[5] made the crucial discovery of the electron by correctly interpreting his measurement of the m/e ratio of cathode rays in terms of a new state of particulate matter "from which all chemical elements are built up". Within three years of this discovery, Paul Drude[6] had synthesized these ideas and had argued, based on the idea of a classical gas of charged electrons, that electrons would exhibit a mean-free path $l = v_{\text{electron}}\tau$, where τ is the scattering rate an l the average distance between scattering events. In Drude's theory electrons were envisioned as diffusing through the metal, and he was able to derive his famous formula for the conductivity σ

$$\sigma = \frac{ne^2\tau}{m}.$$

Missing from Drude's pioneering picture, was any notion of the Fermi-Dirac statistics of the electron fluid. He had for example, no notion that the characteristic velocity of the electrons was given by the Fermi velocity, $v_{\text{electron}} \sim v_F$ a vastly greater velocity at low temperatures than could ever be expected on the grounds of a Maxwell Boltzman fluid of particles. This raises the question - how - in a fully quantum mechanical picture of the electron fluid, can we rederive Drude's basic model?

A real metal contains both disorder and electron-electron interactions - in this course we shall only touch on the simpler problem of disorder in an otherwise free electron gas. We shall actually return to this problem in earnest in the next chapter. Our task here in our first example will be to examine the electron propagator in a disordered medium of elastically scattering impurities. We shall consider an electron in a disordered potential

$$\begin{aligned} H &= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + V_{\rm disorder} \\ V_{\rm disorder} &= \int d^3x U(\vec{x}) \psi^\dagger(\mathbf{x}) \psi^\dagger(\mathbf{x}) \end{aligned} \tag{9.77}$$

where $U(\mathbf{x})$ represents the scattering potential generated by a random array of N_i impurities located at positions $\mathbf{R_j}$, each with atomic potential $\mathcal{U}(\mathbf{x}-\mathbf{R_j})$,

$$U(\mathbf{x}) = \sum_j \mathcal{U}(\mathbf{x}-\mathbf{R_j})$$

An important aspect of this Hamiltonian, is that it contains no interactions between electrons, and as such the energy of each individual electron is conserved: all interactions are elastic.

We shall not be interested in calculating the value of a physical quantity for a *specific* location of impurities, but rather on the value of that quantity after we have averaged over the locations of the impurities, i.e.

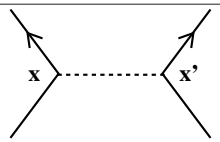
$$\overline{\langle A\rangle} = \int \prod_j \frac{1}{V}\, d^3R_j \langle \hat{A}[\{\mathbf{R}_j\}]\rangle$$

This is an elementary example of a "quenched average", in which the "impurity average" takes place *after* the Thermodynamic average. Here, we'll calculate the impurity averaged Green function. To do this we need to know something about the fluctuations of the impurity scattering potential about its average. It is these fluctuations that scatter the electrons.

Electrons will in general scatter off the fluctuations in the potential. The average impurity potential $\overline{U(\mathbf{x})}$ plays the roll of a kind of shifted chemical potential. Indeed, if we shift the chemical potential by an amount $\Delta\mu$, the scattering potential becomes $U(\mathbf{x})-\Delta\mu$, and we can always choose $\Delta\mu$ so that $\overline{U(\mathbf{x})}-\mu = 0$. The more important quantity are the fluctuations about the average potential $\delta U(\mathbf{x}) = U(\mathbf{x}) - \overline{U(\mathbf{x})}$. These fluctuations are spatially correlated, with variance

$$\overline{\delta U(\mathbf{x})\delta U(\mathbf{x}')} = \int_q e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')} n_i\, |u(\mathbf{q})|^2 \tag{9.78}$$

where $u(\mathbf{q}) = \int d^3x \mathcal{U}(\mathbf{x}) e^{-i\mathbf{q}\cdot\mathbf{x}}$ is the Fourier transform of the scattering potential and $n_i = N_i/V$ is the concentration of impurities. It is these fluctuations that scatter the electrons, and when we come to draw the impurity averaged Feynman diagrams, we'll see that the spatial correlations in the potential fluctuations induce a sort of "attractive interaction", denoted by the diagram



$$\int n_i |u(\mathbf{q})|^2 e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')} = -V_{\rm eff}(\mathbf{x}-\mathbf{x}') \tag{9.79}$$

Although in principle, we should keep all higher moments of the impurity scattering potential, in practice, the leading order moments are enough to extract a lot of the basic physics in weakly disordered metals. Notice that the fluctuations in the scattering potential are short-range - they only extend over the range of the scattering potential. Indeed, if we neglect the momentum dependence of $u(\mathbf{q})$, assuming that the impurity scattering is dominated by low energy s-wave scattering, then we can write $u(\mathbf{q}) = u_0$. In this situation, the fluctuations in the impurity scattering potential are entirely local,

$$\overline{\delta U(\mathbf{x})\delta U(\mathbf{x}')} = n_i u_0^2 \delta(\mathbf{x}-\mathbf{x}') \qquad \text{white noise potential}$$

In our discussion today, we will neglect the higher order moments of the scattering potential, effectively assuming that it is purely Gaussian.

To prove (9.78), we first Fourier transform the potential

$$U(\mathbf{q}) = \sum_j e^{-i\mathbf{q}\cdot\mathbf{R_j}} \int d^3x\, \mathcal{U}(\mathbf{x}-\mathbf{R_j}) \mathbf{e}^{-\mathbf{i}\mathbf{q}\cdot(\mathbf{x}-\mathbf{R_j})} = \mathbf{u}(\mathbf{q}) \sum_{\mathbf{j}} \mathbf{e}^{-\mathbf{i}\mathbf{q}\cdot\mathbf{R_j}}, \tag{9.80}$$

so that the locations of the impurities are encoded in the phase shifts which multiply $u(\mathbf{q})$. If we now carry out the average,

$$\begin{aligned} \overline{\delta U(\mathbf{x})\delta U(\mathbf{x}')} &= \int_{\mathbf{q},\mathbf{q}'} e^{i(\mathbf{q}\cdot\mathbf{x}-\mathbf{q}\cdot\mathbf{x}')} \left(\overline{U(\mathbf{q})U(-\mathbf{q}')} - \overline{U(\mathbf{q})}\ \overline{U(-\mathbf{q}')}\right) \\ = \int_{\mathbf{q},\mathbf{q}'} e^{i(\mathbf{q}\cdot\mathbf{x}-\mathbf{q}\cdot\mathbf{x}')} & \quad u(\mathbf{q})u(-\mathbf{q}') \sum_{i,j} \left(\overline{e^{-i\mathbf{q}\cdot\mathbf{R_i}} e^{i\mathbf{q}'\cdot\mathbf{R_j}}} - \overline{e^{-i\mathbf{q}\cdot\mathbf{R_i}}}\ \overline{e^{i\mathbf{q}'\cdot\mathbf{R_j}}}\right) \end{aligned} \tag{9.81}$$

Now since the phase terms are independent at different sites, the variance of the random phase term in the above expression vanishes unless $i=j$, so

$$\begin{aligned} \sum_{i,j} \left(\overline{e^{-i\mathbf{q}\cdot\mathbf{R}_i} e^{i\mathbf{q}'\cdot\mathbf{R}_j}} - \overline{e^{-i\mathbf{q}\cdot\mathbf{R_i}}}\ \overline{e^{i\mathbf{q}'\cdot\mathbf{R_j}}}\right) &= N_i \times \int \frac{1}{V} d^3R_j e^{-i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{R}_j} \\ &= n_i (2\pi)^3 \delta^{(3)}(\mathbf{q}-\mathbf{q}') \end{aligned} \tag{9.82}$$

from which

$$\overline{U(\mathbf{q})U(-\mathbf{q}')} - \overline{U(\mathbf{q})}\ \overline{U(-\mathbf{q}')} = n_i |u(\mathbf{q})|^2 (2\pi)^3 \delta^{(3)}(\mathbf{q}-\mathbf{q}')$$

and (9.78) follows.

Now let us examine how electrons scatter off these fluctuations. If we substitute $\psi^\dagger(\mathbf{x}) = \int_{\mathbf{k}} c^\dagger{}_k e^{-i\mathbf{k}\cdot\mathbf{x}}$ into $\hat{V}_{\rm disorder}$, we obtain

$$\hat{V}_{\rm disorder} = \int_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}} c_{\mathbf{k}'} \delta U(\mathbf{k}-\mathbf{k}')$$

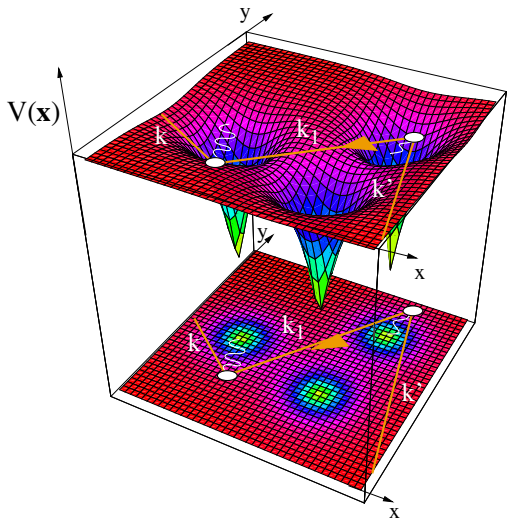
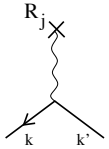


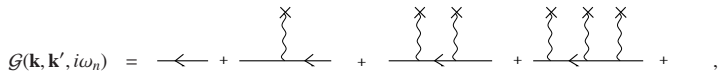
Figure 9.4: Double scattering event in the random impurity potential.

We shall represent the scattering amplitude for scattering once



$$\delta U(\mathbf{k}-\mathbf{k}') = \left(u(\mathbf{k}-\mathbf{k}')\sum_j e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}\right) - \Delta\mu\delta_{\mathbf{k}-\mathbf{k}'}. \tag{9.83}$$

where we have subtracted the scattering off the average potential. The potential transfers momentum, but does not impart any energy to the electron, and for this reason frequency is conserved along the electron propagator. Let us now write down, in momentum space the Greens function of the electron



$$\begin{aligned} &= \mathcal{G}^0(\mathbf{k},i\omega_n)\delta_{\mathbf{k},\mathbf{k}'} + \mathcal{G}^0(\mathbf{k},i\omega_n)\delta U(\mathbf{k}-\mathbf{k}')\mathcal{G}^0(\mathbf{k}',i\omega_n) \\ &+ \int_{\mathbf{k}_1}\mathcal{G}^0(\mathbf{k},i\omega_n)\delta U(\mathbf{k}-\mathbf{k}_1)\mathcal{G}^0(\mathbf{k}_1,i\omega_n)\delta U(\mathbf{k}_1-\mathbf{k}')\mathcal{G}^0(\mathbf{k}',i\omega_n)+\ldots \end{aligned} \tag{9.84}$$

where the frequency $i\omega_n$ is constant along the electron line. Notice that $\mathcal{G}$ is actually a function of each impurity position! Fig. 9.4 illustrates one of the scattering events contributing to the third diagram in this sum. We want to calculate the quenched avaerage $\overline{\mathcal{G}(\mathbf{k},\mathbf{k}',i\omega_n)}$, and to do this, we need to average each Feynman diagram in the above series.

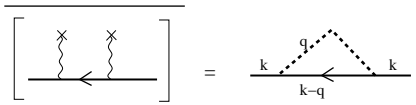
When we impurity average the single scattering event, it vanishes:

$$\overline{\mathcal{G}^0(\mathbf{k},i\omega_n)\delta U(\mathbf{k}-\mathbf{k}')\mathcal{G}^0(\mathbf{k}',i\omega_n)} = \mathcal{G}^0(\mathbf{k},i\omega_n)\overbrace{\overline{\delta U(\mathbf{k}-\mathbf{k}')}}^{=0}\mathcal{G}^0(\mathbf{k}',i\omega_n)$$

but the average of a double scattering event is

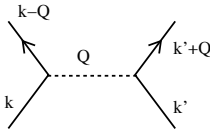
$$\begin{aligned} \sum_{\mathbf{k}_1}\mathcal{G}^0(\mathbf{k},i\omega_n)\mathcal{G}^0(\mathbf{k}_1,i\omega_n)\mathcal{G}^0(\mathbf{k}',i\omega_n)\times\overbrace{\overline{\delta U(\mathbf{k}-\mathbf{k}_1)\delta U(\mathbf{k}_1-\mathbf{k}')}}^{n_i|u_{\mathbf{k}-\mathbf{k}'}|^2\delta_{\mathbf{k}-\mathbf{k}'}} \\ = \delta_{\mathbf{k}-\mathbf{k}'}\times\mathcal{G}^0(\mathbf{k},i\omega_n)^2 n_i\sum_{\mathbf{k}_1}u(\mathbf{k}-\mathbf{k}_1)^2\mathcal{G}^0(\mathbf{k}_1,i\omega_n)\mathcal{G}^0(\mathbf{k},i\omega_n) \end{aligned} \tag{9.85}$$

Notice something fascinating - after impurity averaging, momentum is now conserved. We can denote the impurity averaged double scattering event Feynman diagram



(9.86)

where we have introduced the Feynman diagram



$$n_i|u(\mathbf{q})|^2 = -V_{\rm eff}(Q) \tag{9.87}$$

to denote the momentum transfer produced by the quenched fluctuations in the random potential. In writing the diagram this way, we bring out the notion that quenched disorder can be very loosely thought of as an interaction with an effective potential

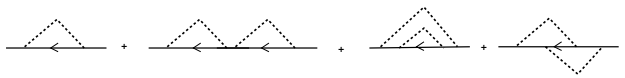
$$V_{\rm eff}(\mathbf{q},i\nu_n) = \int_0^\beta d\tau e^{i\nu_n\tau}\overbrace{\overline{V_{\rm eff}(\mathbf{q},\tau)}}^{-n_i|u(\mathbf{q})|^2} = -\beta\delta_{n0}n_i|u(\mathbf{q})|^2$$

where the $\beta\delta_{n0} \equiv \int d\tau e^{i\nu_n\tau}$ is derived from the fact that the interaction $V_{\rm eff}(\mathbf{q},\tau)$does not depend on the time difference guarantees that there is no energy transferred by the quenched scattering events. In otherwords, quenched disorder induces a sort of infinitely retarded, but "*attractive*" potential between electrons. (Our statement can be made formally correct in the language of replicas - this interaction takes place between electrons of the same, or different replica index. In the $n \to 0$ limit, the residual interaction only acts on one electron in the same replica.) The notion that disorder induces interactions is an interesting one, for it motivates the idea that disorder can lead to new kinds of collective behavior.

After the impurity averaging, we notice that momentum is now conserved, so that the impurity averaged Green function is now diagonal in momentum space,

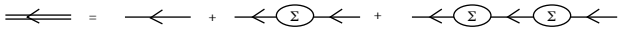
$$\overline{\mathcal{G}(\mathbf{k},\mathbf{k}',i\nu_n)} = \delta_{\mathbf{k}-\mathbf{k}'}\mathcal{G}(\mathbf{k},i\nu_n).$$

If we now carry out the impurity averaging on multiple scattering events, only repeated scattering events at the same sites will give rise to non-vanishing contributions. If we take account of all scattering events induced by the Gaussian fluctuations in the scattering potential, then we generate a series of diagrams of the form

$G(k) =$ 

In the Feynman diagrams, we can group all scatterings into connected self-energy diagrams, as follows:

$\Sigma(k) =$ 

$G(k) =$ 

$$= [i\omega_n - \epsilon_{\mathbf{k}} - \Sigma(k)]^{-1} \tag{9.88}$$

In the case of s-wave scattering, all momentum dependence of the scattering processes is lost, so that in this case $\Sigma(k) = \Sigma(i\omega_n)$ only depends on the frequency. In the above diagram, the double line on the electron propagator indicates that all self-energy corrections have been included. From the above, you can see that the self-energy corrections calculated from the first expression are fed into the electron propagator, which in turn is used in a self-consistent way inside the self-energy

We shall begin by trying to calculate the first order above diagrams for the self-energy without imposing any self-consistency. This diagram is given by

$\Sigma(i\omega_n) =$ 

$$= n_i \sum_{\mathbf{k}'} |u(\mathbf{k}-\mathbf{k}')|^2 G(\mathbf{k}',i\omega_n)$$

$$= n_i \sum_{\mathbf{k}'} |u(\mathbf{k}-\mathbf{k}')|^2 \frac{1}{i\omega_n - \epsilon_{\mathbf{k}'}} \tag{9.89}$$

Now we can replace the summation over momentum inside this self-energy by an integration over solid angle and energy, as follows

$$\sum_{\mathbf{k}'} \to \int \frac{d\Omega_{\mathbf{k}'}}{4\pi} d\epsilon' N(\epsilon')$$

where $N(\epsilon)$ is the density of states. With this replacement,

$$\Sigma(i\omega_n) = n_i u_0^2 \int d\epsilon N(\epsilon) \frac{1}{i\omega_n - \epsilon}$$

where

$$u_0^2 = \int \frac{d\Omega_{\mathbf{k}'}}{4\pi} |u(\mathbf{k}-\mathbf{k}')|^2 = \frac{1}{2}\int_{-1}^{1} d\cos\theta |u(\theta)|^2$$

is the angular average of the squared scattering amplitude. To a good approximation, this expression can be calculated by replacing the energy dependent density of states by its value at the Fermi energy. In so doing, we neglect a small real part to the self-energy, which can, in any case be absorbed by the chemical potential. This kind of approximation is extremely common in many body physics, in cases where the key physics is dominated by electrons close to the Fermi energy. The deviations from constancy in $N(\epsilon)$, will in practice affect the real part of $\Sigma(i\omega_n)$, and these small changes can be accomodated by a shift in the chemical potential. The resulting expression for $\Sigma(i\omega_n)$ is then

$$\Sigma(i\omega_n) = n_i u_0^2 N(0) \int_{-\infty}^{\infty} d\epsilon \frac{1}{i\omega_n - \epsilon} = -i\frac{1}{2\tau}\mathrm{sgn}(\omega_n) \tag{9.90}$$

where we have identified $\frac{1}{\tau} = 2\pi n_i u_0^2$ as the electron elastic scattering rate. We notice that this expression is entirely imaginary, and it only depends on the sign of the Matsubara frequency. Notice that in deriving this result we have extended the limits of integration to infinity, an approximation that involves neglecting terms of order $1/(\epsilon_F\tau)$.

We can now attempt to recompute $\Sigma(i\omega_n)$ with self-consistency. In this case,

$\Sigma(i\omega_n) =$ 

$$= n_i u_0^2 \sum_{\mathbf{k}'} \frac{1}{i\omega_n - \epsilon_{\mathbf{k}'} - \Sigma(i\omega_n)} \tag{9.91}$$

If carry out the energy integration again, we see that the imposition of self-consistency has no effect on the scattering rate

$$\begin{aligned}\Sigma(i\omega_n) &= n_i u_0^2 N(0) \int_{-\infty}^{\infty} d\epsilon \frac{1}{i\omega_n - \epsilon - \Sigma(i\omega_n)} \\ &= -i\frac{1}{2\tau}\mathrm{sgn}(\omega_n).\end{aligned} \tag{9.92}$$

Our result for the electron propagator, ignoring the "vertex corrections" to the scattering self-energy is given by

$$G(\mathbf{k}, z) = \frac{1}{z - \epsilon_{\mathbf{k}} + i\frac{1}{2\tau}\mathrm{sgn}Im(z)}$$

where we have boldly extended the Green function into the complex plane. We may now make a few remarks:

- The original pole of the Green function has been broadened. The electron "spectral function",

$$A(\mathbf{k}, \omega) = \frac{1}{\pi}\mathrm{Im}G(\mathbf{k}, \omega - i\delta) = \frac{1}{\pi}\frac{(2\tau)^{-1}}{(\omega - \epsilon_{\mathbf{k}})^2 + (2\tau)^{-2}}$$

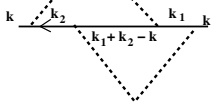
  is a Lorentzian of width $1/\tau$. The electron of momentum $\mathbf{k}$ now has a lifetime τ due to elastic scattering effects.

- Although the electron has a mean-free path, $l = v_F\tau$the electron propagator displays no features of diffusion. The main effect of the finite scattering rate is to introduce a decay length into the electron propagation. The electron propagator does not bear any resemblance to the "diffusion propagator" $\chi = 1/(iv - Dq^2)$ that is the Greens function for the diffusion equation $(\partial_t - D\nabla^2)\chi = -\delta(x, t)$. The physics of diffusion and Ohm's law do not appear until we are able to examine the charge and spin response functions, and for this, we have to learn how to compute the density and current fluctuations in thermal equilibrium. (Chapter 10).

- The scattering rate that we have computed is often called the "classical" electron scattering rate. The neglected higher order diagrams with vertex corrections are actually smaller than the leading order contribution by an amount of order

$$\frac{1}{\epsilon_F\tau} = \frac{1}{k_F l}$$

  This small parameter defines the size of "quantum corrections" to the Drude scattering physics, which are the origin of the physics of electron localization. To understand how this small number arises in the self-energy, consider the first vertex correction to the impurity scattering,



(9.93)

  This diagram is given by

$$\Sigma_2 = \overbrace{N(0)\int\frac{d\epsilon_1}{i\omega_n - \epsilon_1}}^{-i\frac{1}{2\tau}}\overbrace{N(0)\int\frac{d\epsilon_2}{i\omega_n - \epsilon_2}}^{-i\frac{1}{2\tau}}\overbrace{\int\frac{d\Omega_1 d\Omega_2}{(4\pi)^2}\frac{1}{i\omega_n - \epsilon_{\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}}}}^{\sim\frac{-i}{k_F v_F}}$$

$$\sim \; i\frac{1}{\tau}\times\frac{1}{k_F l} \tag{9.94}$$

where the last term in the integral derives from the central propagator in the self-energy. In this self-energy, the momentum of the central propagator is entirely determined by the momentum of the two other internal legs, so that the energy associated with this propagator is $\epsilon_{-\mathbf{k}+\mathbf{k}_1+\mathbf{k}_2}$. This energy is only close to the Fermi energy when $\mathbf{k}_1 \sim -\mathbf{k}_2$, so that only a small fraction $1/(k_F l)$ of the possible directions of k_2 give a large contribution to the scattering processes.

9.7 Interacting electrons and phonons

The electron phonon interaction is one of the earliest successes of many body physics in condensed matter. In many ways, it is the condensed matter analog of quantum-electrodynamics - and the early work on the electron phonon problem was carried out by physicists who had made their early training in the area of quantum electrodynamics.

When an electron passes through a crystal, it attracts the nearby ions, causing a local build-up of positive charge. Perhaps a better analogy, is with a supersonic aircraft, for indeed, an electron is a truly supersonic particle inside crystals, moving at many times the velocity of sound. To get an idea of just how much faster the electron moves in comparison with sound, notice that the ratio of the sound velocity v_s to the Fermi velocity $v_F$is determined by the ratio of the Debye frequency to the Fermi energy, for

$$\frac{v_s}{v_F} \sim \frac{\nabla_k\omega_k}{\nabla_k\epsilon_k} \sim \frac{\omega_D/a}{\epsilon_F/a} = \frac{\omega_D}{\epsilon_F}$$

where a is the size of the unit cell. Now an approximate estimate for the Debye frequency is given by $\omega_D^2 \sim k/M$, where M is the mass of an atomic nucleus and $k \sim \epsilon_F/a^2$ is the "spring constant" associated with atomic motions, thus

$$\omega_D^2 \sim \left(\frac{\epsilon_F}{a^2}\right)\frac{1}{M}$$

and

$$\frac{\omega_D^2}{\epsilon_F^2} \sim \underbrace{\frac{1}{(\epsilon_F a^2)}}_{\sim 1/m}\frac{1}{M} \sim \frac{m}{M}$$

so that the ratio

$$\frac{v_s}{v_F} \sim \sqrt{\frac{m}{M}} \sim \frac{1}{100}.$$

so an electron moves at around Mach 100. As it moves through the crystal, it leaves behind it a very narrow wake of "positively charged" distortion in the crystal lattice which attracts other electrons, long after the original disturbance has passed by. This is the origin of the weak attractive interaction produced by the exchange of virtual phonons. This attractive interaction is highly retarded, quite unlike the strongly repulsive Coulomb interaction that acts between electrons which is almost instantaneous in time. (The ratio of characteristic timescales being $\sim \frac{\epsilon_F}{\omega_D} \sim \sqrt{\frac{M}{m}} \sim 100$). Thus-

whereas two electrons at the same place and time, feel a strong mutual Coulomb repulsion, two electrons which arrive at the same place, but at different times can be subject to an attractive electron phonon interaction. It is this interaction that is responsible for the development of superconductivity in many conventional metals.

In an electron fluid, we must take into account the quantum nature of the sound-vibrations. An electron can not continously interact with the surrounding atomic lattice - it must do so by the emission and absorption of sound quanta or "phonons". The basic Hamiltonian to describe the electron phonon problem is the Frohlich Hamiltonian, derived by Fröhlich, a German emigré to Britain, who worked in Liverpool shortly after the second-world war[7]. Fröhlich recognized that the electron-phonon interaction is closely analogous to the electron-photon interaction of QED. Fröhlich appreciated that this interaction would give rise to an effective attraction between electrons and he was the first to identify it as the driving force behind conventional superconductivity.

To introduce the Frohlich Hamiltonian, we will imagine we have a three phonon modes labelled by the index $\lambda = (1, 2, 3)$, with frequency $\omega_{\mathbf{q}\lambda}$. For the moment, we shall also ignore the Coulomb interaction between electrons. The Fröhlich Hamiltonian is then

$$\begin{aligned} H_e &= \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \\ H_p &= \sum_{\mathbf{q},\lambda} \omega_{\mathbf{q}\lambda} (a^\dagger_{\mathbf{q}\lambda} a_{\mathbf{q}\lambda} + \frac{1}{2}) \\ H_I &= \sum_{\mathbf{k},\mathbf{q},\lambda} g_{\mathbf{q}\lambda} c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma} \left[a_{\mathbf{q}\lambda} + a^\dagger_{-\mathbf{q}\lambda} \right] \end{aligned} \tag{9.95}$$

To understand the electron phonon coupling, let us consider how long-wavelength fluctuations of the lattice couple to the electron energies. Let $\vec{\Phi}(\mathbf{x})$ be the displacement of the lattice at a given point $\mathbf{x}$, so that the strain tensor in the lattice is given by

$$u_{\mu\nu}(\mathbf{x}) = \frac{1}{2}\left(\nabla_\mu \Phi_\nu(\mathbf{x}) + \nabla_\nu \Phi_\mu(\mathbf{x})\right)$$

In general, we expect a small change in the strain to modify the background potential of the lattice, modifying the energies of the electrons, so that locally,

$$\epsilon(\mathbf{k}) = \epsilon_0(\mathbf{k}) + C_{\mu\nu} u_{\mu\nu}(\mathbf{x}) + \ldots$$

Consider the following, very simple model. In a free electron gas, the Fermi energy is related to the density of the electrons N/V by

$$\epsilon_F = \frac{1}{2m}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}}. \tag{9.96}$$

When a portion of the lattice expands from $V \to V + dV$, the positive charge of the background lattice is unchanged, and preservation of overall charge neutrality guarantees that the number of

electrons N remains constant, so the change in the Fermi energy is given by

$$\frac{\delta\epsilon_F}{\epsilon_F} = -\frac{2}{3}\frac{dV}{V} \sim -\frac{2}{3}\vec{\nabla}\cdot\vec{\Phi}$$

On the basis of this simple model, we expect the following coupling between the displacement vector and the electron field

$$H_I = C\int d^3x \psi_\sigma{}^\dagger(\mathbf{x})\psi_\sigma(\mathbf{x})\vec{\nabla}.\vec{\Phi} \qquad C = -\frac{2}{3}\epsilon_F \tag{9.97}$$

The quantity C is often called the "deformation potential". Now the displacement of the the phonons was studied in Chapter 4. In a general model, it is given by

$$\Phi(\mathbf{x}) = -i\sum_{\mathbf{q},\lambda} \mathbf{e}^\lambda_{\mathbf{q}}\, \Delta x_{\mathbf{q}\lambda}\left[a_{\mathbf{q}\lambda} + a^\dagger_{-\mathbf{q}\lambda}\right] e^{i\mathbf{q}\cdot\mathbf{x}}$$

where we've introduced the shorthand

$$\Delta x_{\mathbf{q}\lambda} = \left(\frac{\hbar}{2MN_s\omega_{\mathbf{q}\lambda}}\right)^{\frac{1}{2}}$$

to denote the characteristic zero point fluctuation associated with a given mode. (N_s is the number of sites in the lattice.) The body of this expression is essentially identical to the displacement of a one-dimensional harmonic lattice (see (3.81)), dressed up with additional polarization indices. The unfamiliar quantity $\mathbf{e}^\lambda_{\mathbf{q}}$ is the polarization vector of the mode. For longitudinal phonons, for instance, $\mathbf{e}^L_{\mathbf{q}} = \hat{q}$. The "$-i$" infront of the expression has been introduced into the definition of the phonon creation and annihilation operators so that the requirement that the Hamiltonian is hermitian (which implies $(\mathbf{e}^\lambda_{\mathbf{q}})^* = -(\mathbf{e}^\lambda_{-\mathbf{q}})$) is consistent with the convention that $\mathbf{e}$ changes sign when the momentum vector $\mathbf{q}$ is inverted.

The divergence of the phonon field is then

$$\vec{\nabla}\cdot\Phi(\mathbf{x}) = \sum_{\mathbf{q},\lambda} \mathbf{q}\cdot\mathbf{e}^\lambda_{\mathbf{q}}\Delta x_{\mathbf{q}\lambda}\left[a_{\mathbf{q}\lambda} + a^\dagger_{-\mathbf{q}\lambda}\right] e^{i\mathbf{q}\cdot\mathbf{x}}$$

In this simple model, the electrons only couple to the longitudinal phonons, since these are the only phonons that change the density of the unit cell. When we now Fourier transform the interaction Hamiltonian, making the insertion $\psi_\sigma(\mathbf{x}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} c_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{x}}$ (9.97), we obtain

$$\begin{aligned} H_I &= C\int d^3x \psi_\sigma{}^\dagger(\mathbf{x})\psi_\sigma(\mathbf{x})\vec{\nabla}\cdot\vec{\Phi}(\mathbf{x}) \\ &= \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\lambda} c^\dagger_{\mathbf{k}'\sigma} c_{\mathbf{k}\sigma}\left[a_{\mathbf{q}\lambda} + a^\dagger_{-\mathbf{q}\lambda}\right] \overbrace{\frac{1}{V}\int d^3x e^{i(\mathbf{q}+\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}}^{\delta_{\mathbf{k}'-(\mathbf{k}+\mathbf{q})}} \times C\Delta x_{\mathbf{q}\lambda}(\mathbf{q}\cdot\mathbf{e}^\lambda_{\mathbf{q}}) \end{aligned}$$

$$= \sum_{\mathbf{q}\mathbf{k}\lambda} g_{\mathbf{q}\lambda} c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma} \left[a_{\mathbf{q}\lambda} + a^\dagger_{-\mathbf{q}\lambda} \right] \tag{9.98}$$

where

$$g_{\mathbf{q}\lambda} = \begin{cases} Cq\Delta x_{\mathbf{q}\lambda} = Cq\left(\frac{\hbar}{2MN_s\omega_{\mathbf{q}\lambda}}\right)^{\frac{1}{2}} & (\lambda = L) \\ 0 & (\text{otherwise}) \end{cases}$$

Note that $N_s = V/a^3$, where a is the lattice spacing. To go over to the thermodynamic limit, we will replace our discrete momentum sums by continuous integrals, $\sum_{\mathbf{q}} \equiv V \int_{\mathbf{q}} \to \int_{\mathbf{q}}$. Rather than spending a lot of time keeping track of how the volume factor is absorbed into the integrals, it is simpler to regard $V = 1$ as a unit volume, replacing $N_s \to a^{-3}$ whenever we switch from discrete, to continuous integrals. With this understanding, we will use

$$g_{\mathbf{q}} = Cq\sqrt{\hbar a^3/(2M\omega_{\mathbf{q}\lambda})} \tag{9.99}$$

for the electron-phonon coupling to the longitudinal modes. Our simple model captures the basic aspects of the electron phonon interaction, and it can be readily generalized. In a more sophisticated model,

- C becomes momentum dependent and should be replaced by the Fourier transform of the atomic potential. For example, if we compute the electron - phonon potential from given by the change in the atomic potential V_{atomic} resulting from the displacement of atoms,

$$\delta V(\mathbf{x}) = \sum_j \delta V_{\text{atomic}}(\mathbf{x} - \mathbf{R}^0_j - \vec{\Phi}_j) = -\sum_j \vec{\Phi}_j \cdot \vec{\nabla} V_{\text{atomic}}(\mathbf{x} - \mathbf{R}^0_j)$$

  we must replace interaction,

$$C \to V_{\text{atomic}}(\mathbf{q}) = \frac{1}{v_{cell}} \int d^3x V_{\text{atomic}}(\mathbf{x}) e^{-i\mathbf{q}\cdot\mathbf{x}}. \tag{9.100}$$

- When the plane-wave functions are replaced by the detailed Bloch wavefunctions of the electron band, the electron phonon coupling becomes dependent on both the incoming and outgoing electron momenta, so that

$$g_{\mathbf{k}'-\mathbf{k}\lambda} \to g_{\mathbf{k}',\mathbf{k}\lambda}.$$

Nevertheless, much can be learnt from our simplified model In the discussion that follows, we shall drop the polarization index, and assume that the phonon modes we refer to are exclusively longitudinal modes.

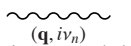
In setting up the Feynman diagrams for our Frohlich model, we need to introduce two new elements- a diagram for the phonon propagator, and a diagram to denote the vertex. If we denote $\phi_{\mathbf{q}} = a_{\mathbf{q}} + a^\dagger_{-\mathbf{q}}$, then the phonon Green function is given by

$$D(\mathbf{q}, \tau - \tau') = -\langle T\phi_{\mathbf{q}}(\tau)\phi_{\mathbf{q}}(\tau')\rangle = T\sum_{i\nu_n} D(q) e^{-i\nu_n(\tau-\tau')} \tag{9.101}$$

where the propagator

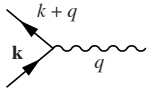
$$D(q) = \frac{2\omega_{\mathbf{q}}}{(i\nu_n)^2 - (\omega_{\mathbf{q}})^2}$$

is denoted by the diagram



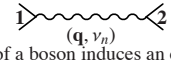
$$= D(\mathbf{q}, i\nu_n) \tag{9.102}$$

The interaction vertex between electrons and phonon is denoted by the diagram



$$= (i)^3 \times -g_{\mathbf{q}} = ig_{\mathbf{q}} \tag{9.103}$$

The factor i^3 arises because we have three propagators entering the vertex, each donating a factor of i. The $-1g_{\mathbf{q}}$ derives from the interaction Hamiltonian in the time-ordered exponential. Combining these two Feynman rules, we see that when two electrons exchange a boson, this gives rise to the diagram



$$= (ig_{\mathbf{q}})^2 D(q) = -(g_{\mathbf{q}})^2 D(q) \tag{9.104}$$

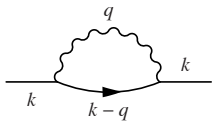
so that the exchange of a boson induces an effective interaction

$$\boxed{V_{\text{eff}}(\mathbf{q}, z) = g^2_{\mathbf{q}} \frac{2\omega_{\mathbf{q}}}{(z)^2 - \omega^2_{\mathbf{q}}}} \tag{9.105}$$

Notice three things about this interaction -

- It is strongly frequency dependent, reflecting the strongly retarded nature of the electron phonon interaction. The characteristic phonon frequency is the Debye frequency ω_D, and the characteristic "restitution" time associated with the electron phonon interaction is $\tau \sim 1/\omega_D$, whereas the corresponding time associated with the repulsive Coulomb interaction is of order $1/\epsilon_F$. The ratio $\epsilon_F/\omega_D \sim 100$ is a measure of how much more retarded the electron-phonon interaction is compared with the Coulomb potential.
- It is weakly dependent on momentum, describing an interaction that is spatially local over one or two lattice spacings.
- At frequencies below the Debye energy, $\omega \lesssim \omega_D$ the denominator in V_{eff} changes sign, and the residual low-energy interaction is actually attractive. It is this component of the interaction that is responsible for superconductivity in conventional superconductors.

We wish to now calculate the effect of the electron-phonon interaction on electron propagation. The main effect on the electron propagation is determined by the electron-phonon self energy. The leading order Feynman diagram for the self-energy is given by



$$\equiv \Sigma(k) = \sum_q (ig_{\mathbf{q}})^2 \mathcal{G}^0(k-q)D(q) \tag{9.106}$$

or written out explicitly,

$$\begin{aligned}\Sigma(\mathbf{k}, i\omega_n) &= -T\sum_{\mathbf{q},iv_n} g_{\mathbf{q}}^2\left[\frac{2\omega_{\mathbf{q}}}{(iv_n)^2-\omega_{\mathbf{q}}^2}\right]\frac{1}{i\omega_n - iv_n - \epsilon_{\mathbf{k}-\mathbf{q}}} \\ &= -T\sum_{\mathbf{q},iv_n}\left[\frac{1}{iv_n-\omega_{\mathbf{q}}}\frac{1}{i\omega_n - iv_n - \epsilon_{\mathbf{k}-\mathbf{q}}} - (\omega_{\mathbf{q}} \to -\omega_{\mathbf{q}})\right]\end{aligned} \tag{9.107}$$

where we have simplified the expression by splitting up the boson propagator into a positive and negative frequency component, the latter being obtained by reversing the sign on $\omega_{\mathbf{q}}$. We shall carry out the Matsubara sum over the bosonic frequencies by writing it as a contour integral with the Bose function:

$$-T\sum_{iv_n} F(iv_n) = -\int_C \frac{dz}{2\pi i} n(z)F(z) = \int_{C'}\frac{dz}{2\pi i}n(z)F(z) \tag{9.108}$$

where C runs anti-clockwise around the imaginary axis and C' runs anticlockwise around the poles in $F(z)$. In this case, we choose

$$\begin{aligned}F(z) &= \frac{1}{z-\omega_{\mathbf{q}}}\frac{1}{i\omega_n - z - \epsilon_{\mathbf{k}-\mathbf{q}}} \\ &= \left[\frac{1}{z-\omega_{\mathbf{q}}} - \frac{1}{z-(i\omega_n - \epsilon_{\mathbf{k}-\mathbf{q}})}\right]\frac{1}{i\omega_n - (\omega_{\mathbf{q}}+\epsilon_{\mathbf{k}-\mathbf{q}})}\end{aligned} \tag{9.109}$$

which has two poles, one at $z = \omega_{\mathbf{q}}$ and one at $z = i\omega_n - \epsilon_{\mathbf{k}-\mathbf{q}}$ (Fig. 9.5). Carrying out the contour

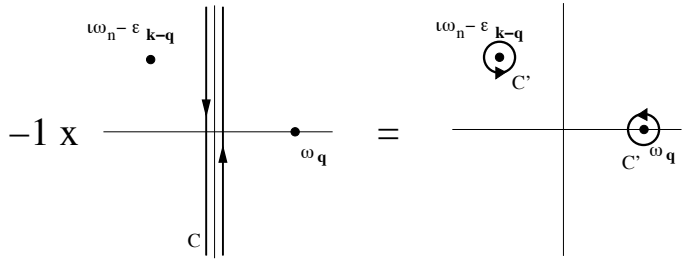


Figure 9.5: Contours C and C' used in evaluation of $\Sigma(\mathbf{k}, i\omega_n)$

integral, we then obtain

$$\begin{aligned}\Sigma(k) &= \sum_{\mathbf{q}} g_{\mathbf{q}}^2\left[\frac{n(\omega_{\mathbf{q}}) - \overbrace{n(i\omega_n - \epsilon_{\mathbf{k}-\mathbf{q}})}^{-(1-f_{\mathbf{k}-\mathbf{q}})}}{i\omega_n - (\omega_{\mathbf{q}}+\epsilon_{\mathbf{k}-\mathbf{q}})} - \{\omega_{\mathbf{q}} \to -\omega_{\mathbf{q}}\}\right] \\ &= \sum_{\mathbf{q}} g_{\mathbf{q}}^2\left[\frac{1+n_{\mathbf{q}} - f_{\mathbf{k}-\mathbf{q}}}{i\omega_n - (\omega_{\mathbf{q}}+\epsilon_{\mathbf{k}-\mathbf{q}})} - \{\omega_{\mathbf{q}} \to -\omega_{\mathbf{q}}\}\right]\end{aligned} \tag{9.110}$$

The second term in this expression is obtained by reversing the sign on $\omega_{\mathbf{q}}$ in the first term, which gives finally,

$$\boxed{\Sigma(\mathbf{k}, z) = \sum_{\mathbf{q}} g_{\mathbf{q}}^2\left[\frac{1+n_{\mathbf{q}} - f_{\mathbf{k}-\mathbf{q}}}{z-(\epsilon_{\mathbf{k}-\mathbf{q}}+\omega_{\mathbf{q}})} + \frac{n_{\mathbf{q}} + f_{\mathbf{k}-\mathbf{q}}}{z-(\epsilon_{\mathbf{k}-\mathbf{q}}-\omega_{\mathbf{q}})}\right]}$$

where we have taken the liberty of analytically extending the function into the complex plane. There is a remarkable amount of physics hidden in this expression.

The terms appearing in the electron phonon self-energy can be interpreted in terms of virtual and real phonon emission processes. Consider the zero temperature limit, when the Bose terms $n_{\mathbf{q}} = 0$. If we look at the first term in $\Sigma(k)$, we see that the numerator is only finite if the intermediate electron state is empty, i.e $|\mathbf{k}-\mathbf{q}| > k_F$. Furthermore, the poles of the first expression are located at energies $\omega_{\mathbf{q}} + \epsilon_{\mathbf{k}-\mathbf{q}}$, which is the energy of an electron of momentum $\mathbf{k}-\mathbf{q}$ and an emitted phonon of momentum $\omega_{\mathbf{q}}$, so the first process corresponds to phonon emission by an electron. If we look at the second term, then at zero temperature, the numerator is only finite if $|\mathbf{k}-\mathbf{q}| < k_F$, so the intermediate state is a hole. The pole in the second term occurs at $-z = -\epsilon_{\mathbf{k}-\mathbf{q}} + \omega_{\mathbf{q}}$, corresponding to a state of one hole and one phonon, so one way to interpret the second term as the energy shift that results from the emission of virtual phonons by holes. At zero temperature then,

$$\Sigma(\mathbf{k}, z) = \sum_{\mathbf{q}} g_{\mathbf{q}}^2\Big[\overbrace{\frac{1-f_{\mathbf{k}-\mathbf{q}}}{z-(\epsilon_{\mathbf{k}-\mathbf{q}}+\omega_{\mathbf{q}})}}^{\text{virtual/real phonon emission by electron}} + \overbrace{\frac{f_{\mathbf{k}-\mathbf{q}}}{z-(\epsilon_{\mathbf{k}-\mathbf{q}}-\omega_{\mathbf{q}})}}^{\text{virtual/real phonon emission by hole}}\Big]$$

As we shall discuss in more detail in the next chapter, the analytically extended Greens function

$$G(\mathbf{k}, z) = \frac{1}{z - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, z)}$$

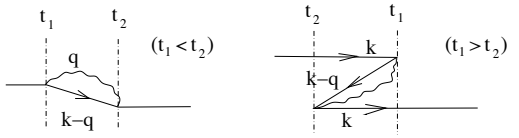
can be used to derive the real-time dynamics of the electron in thermal equilibrium. In general, $\Sigma(\mathbf{k}, \omega - i\delta) = Re\Sigma(\mathbf{k}, \omega - i\delta) + iIm\Sigma(\mathbf{k}, \omega - i\delta)$ will have a real and an imaginary part. The solution of the relation

$$\epsilon_{\mathbf{k}}^* = \epsilon_{\mathbf{k}} + Re\Sigma(\mathbf{k}, \epsilon_{\mathbf{k}}^*)$$

determines the renormalized energy of the electron due to virtual phonon emission. Let's consider the case of an electron, for which $\epsilon^*_{\mathbf{k}}$ is above the Fermi energy. The quasiparticle energy takes the form

$$\epsilon^*_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \overbrace{\sum_{|\mathbf{k}-\mathbf{q}|>k_F} g^2_{\mathbf{q}} \frac{1}{(\epsilon_{\mathbf{k}-\mathbf{q}}+\omega_{\mathbf{q}})-\epsilon^*_{\mathbf{k}}}}^{\text{energy lowered by virtual phonon emission}} + \overbrace{\sum_{|\mathbf{k}-\mathbf{q}|<k_F} g^2_{\mathbf{q}} \frac{1}{\epsilon^*_{\mathbf{k}}+|\epsilon_{\mathbf{k}-\mathbf{q}}|+\omega_{\mathbf{q}}}}^{\text{energy raised by blocking vacuum fluctuations}}.$$

If we approximate $\epsilon^*_{\mathbf{k}}$ by its unrenormalized value $\epsilon_{\mathbf{k}}$, we obtain the second-order perturbation correction to the electron quasiparticle energy, due to virtual phonon processes. To understand these two terms, it is helpful to redraw the Feynman diagram for the self energy so that the scattering events are explicitly time ordered, then we see that there are two virtual processes - depending on whether the intermediate electron line propagates forwards or backwards in time:



Virtual phonon emission Virtual phonon and e–h pair

The first term is recognized as the effect of virtual scattering into an intermediate state with one photon and one electron. But what about the second term? This term involves the initial formation of an electron-hole pair and the subsequent reannihilation of the hole with the incoming electron. During the intermediate process, there seem to be *two* electrons (with the same spin) in the same momentum state $\mathbf{k}$. Can it really be that virtual processes violate the exculsion principle? Fortunately, another interpretation can be given. Under close examination, we see that unlike typical virtual fluctuations to high energy states, which lower the total energy, this term actually raises the quasiparticle energy. These energy raising processes are a "blocking effect" produced by the exclusion principle, on the vacuum fluctuations. In the ground-state, there are virtual fluctuations

$$GS \rightleftharpoons \text{electron } (\mathbf{k}') + \text{hole } (-\mathbf{k}' - \mathbf{q}) + \text{phonon } (\mathbf{q})$$

which lower the energy of the ground-state. When a single electron occupies the state of momentum $\mathbf{k}$, the exclusion principle prevents vacuum fluctuations with $\mathbf{k}' = \mathbf{k}$, raising the energy of the quasiparticle. So time ordered diagrams that appear to violate the exclusion principle describe the suppression of vacuum fluctuations by the exclusion principle.

If we now extend our discussion to finite temperatures, for any given $\mathbf{k}$ and $\mathbf{q}$, both the first and the second terms in the phonon self-energy are present. For phonon emission processes, the appearance of the additional Bose terms $n_{\mathbf{q}}$ is the the effect of stimulated emission, whereby the occupancy of phonon states enhances the emission of phonons. The terms which vanish at zero temperature can also be interpreted as the effect of phonon absorption of the now thermally excited

phonons, i.e

$$\Sigma(\mathbf{k},z) = \sum_{\mathbf{q}} g^2_{\mathbf{q}} \Big[\underbrace{\frac{1-f_{\mathbf{k}-\mathbf{q}}+n_{\mathbf{q}}}{z-(\epsilon_{\mathbf{k}-\mathbf{q}}+\omega_{\mathbf{q}})}}_{\text{virtual/real phonon absorption by hole}} + \underbrace{\frac{f_{\mathbf{k}-\mathbf{q}}+n_{\mathbf{q}}}{z-(\epsilon_{\mathbf{k}-\mathbf{q}}-\omega_{\mathbf{q}})}}_{\text{virtual/real phonon absorption by electron}} \Big]$$

By contrast, the imaginary part of the self-energy determines the decay rate of the electron due to real phonon emission, and the decay rate of the electron is related to the quantity

$$\Gamma_{\mathbf{k}} = 2Im\Sigma(\mathbf{k}, \epsilon^*_{\mathbf{k}} - i\delta) \approx 2Im\Sigma(\mathbf{k}, \epsilon_{\mathbf{k}} - i\delta)$$

If we use the Dirac relation

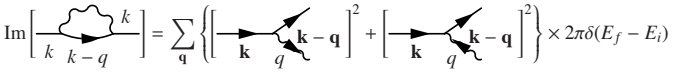
$$\left[\frac{1}{x-a-i\delta}\right] = P\frac{1}{x-a} + i\pi\delta(x-a)$$

then we see that for a weak interaction, the decay rate of the electron is given by

$$\Gamma_{\mathbf{k}} = 2\pi \sum_{\mathbf{q}} g^2_{\mathbf{q}} \Big[\overbrace{(1+n_{\mathbf{q}}-f_{\mathbf{k}-\mathbf{q}})\delta(\epsilon_{\mathbf{k}}-(\epsilon_{\mathbf{k}-\mathbf{q}}+\omega_{\mathbf{q}}))}^{\text{phonon emission}} + \overbrace{(n_{\mathbf{q}}+f_{\mathbf{k}-\mathbf{q}})\delta(\epsilon_{\mathbf{k}}-(\epsilon_{\mathbf{k}-\mathbf{q}}-\omega_{\mathbf{q}}))}^{\text{phonon absorption}} \Big]$$

which we may identify as the contribution to the decay rate from phonon emission and absorption, respectively. Schematically, we may write

$$\text{Im}\left[\quad\right] = \sum_{\mathbf{q}} \left\{ \left[\quad\right]^2 + \left[\quad\right]^2 \right\} \times 2\pi\delta(E_f - E_i)$$



so that taking the imaginary part of the self-energy "cuts" the internal lines. The link between the imaginary part of the self-energy and the real decay processes of absorption and emission is sometimes refered to as the "optical theorem".

9.7.1 α^2F: the electron-phonon coupling function

One of the most important effects of the electron phonon interaction, is to give rise to a superconducting instability. Superconductivity is driven by the interaction of low-energy electrons very close to the Fermi surface, so the amount of energy transferred in an interaction is almost zero. For this reason, the effective interaction between the electrons is given by (9.105)

$$V_{\text{eff}}(\mathbf{q},0) = -\frac{2g^2_{\mathbf{q}}}{\omega_{\mathbf{q}}}$$

Now the momentum dependence of this interaction is very weak. In our simple model, for example, $g^2_{\mathbf{q}}/2\omega_q \sim \frac{q^2}{\omega^2_q} \sim$ constant, and a weak momentum dependence implies that to a first approximation

then, the effective low energy interaction is local, extending over one unit cell and of approximate form

$$H_{eff} \approx -g \sum_{\sigma\sigma'} \sum_{\mathbf{q},\mathbf{k},\mathbf{k}',(|\epsilon_{\mathbf{k}}|,\ |\epsilon_{\mathbf{k}'}|,\ |\epsilon_{\mathbf{k}+\mathbf{q}}|,\ |\epsilon_{k'+\mathbf{q}}|,\ <\omega_D)} \psi^\dagger{}_{\mathbf{k}+\mathbf{q}\sigma}\psi^\dagger{}_{\mathbf{k}'\sigma'}\psi_{\mathbf{k}'+\mathbf{q}\sigma'}\psi_{\mathbf{k}\sigma} \tag{9.111}$$

where the sum over electron momenta is restricted to within a narrow band of energies, within ω_D of the Fermi energy. This means that the interaction is "instantaneous" to within a time-scale of $\delta t \sim 1/\omega_D$. The effective interaction strength g is the sum over all $2g^2_{\mathbf{q}}/\omega_{\mathbf{q}}$,

$$g = \frac{1}{V}\sum_{\mathbf{q}} \frac{2g^2_{\mathbf{q}}}{\omega_{\mathbf{q}}} \equiv \int_{\mathbf{q}} \frac{2g^2_{\mathbf{q}}}{\omega_{\mathbf{q}}} \qquad (V \equiv 1) \tag{9.112}$$

Bardeen and Pines were amongst the first to realize that the electron-electron interaction induced by phonon exchange is highly retarded relative to the almost instantaneous Coulomb interaction, so that for low energy processes, the Coulomb interaction could be ignored. The attractive interaction in (9.111) was then the basis of the "Bardeen-Pines" model[8] - a predecessor of the BCS Hamiltonian. We can make an order-of-magnitude estimate of g, by replacing

$$g \sim \frac{g^2_{2k_F}}{a^3\omega_D} \sim \frac{1}{a^3\omega_D}\overbrace{\left[\left(\frac{a^3}{2M\omega_D}\right)\epsilon_F^2(2k_F)^2\right]}^{(g_{2k_F})^2} \sim \overbrace{\left(\frac{\epsilon_F^2}{\omega_D^2}\right)}^{\frac{M}{m}}\frac{k_F^2}{2M} \sim \epsilon_F$$

where we have taken $\hbar = 1$ and replaced $\int_{\mathbf{q}} \to 1/a^3$. The electron phonon coupling constant is defined as the product of the interaction strength, times the electron density of states,

$$\lambda = N(0)g = \sum_{\mathbf{q}} \frac{2N(0)g^2_{\mathbf{q}}}{\omega_{\mathbf{q}}} \tag{9.113}$$

This dimensionless quantity is not reduced by the small ratio of electron to atom mass, and in typical metals $\lambda \sim 0.1 - 0.2$. We'll now relate the electron phonon self energy to this quantity.

The electron-phonon self-energy can be simplified by the introduction of a function we call "α^2F", that keeps track of the frequency dependence of the electron-phonon coupling constant, where $\alpha(\omega)$ is the typical energy dependent coupling constant and F is the phonon density of states. It turns out that α^2F can be actually measured inside superconductors and F can be measured by neutron scattering.

The basic idea here, is that the momentum dependence of the electron-phonon self energy is far smaller than the frequency dependence, so the momentum dependence of the self-energy can be neglected. The dimensionless ratio between these two dependences is a small number of order ω_D/ϵ_F,

$$\left(\frac{1}{v_F}|\nabla_k\Sigma|\right)/\left(\frac{\partial\Sigma}{\partial\omega}\right) \sim \frac{\omega_D}{\epsilon_F} << 1$$

To a good approximation then, the electron phonon self-energy can be averaged over the Fermi surface, writing

$$\Sigma(\omega) = \frac{\int dS\ \Sigma(\mathbf{k},\omega)}{\int dS}$$

where $\int dS \equiv \int d^2k/(2\pi)^3$ is an integral over the Fermi surface. Now the sum over $\mathbf{k}'$ inside the self-energy can be replaced by a combination of an energy integral, and a Fermi surface integral, as follows

$$\sum_{\mathbf{k}'} \to \int dS' dk'_{\rm perp} = \int \frac{dS'}{|d\epsilon_{k'}/dk'|}d\epsilon' = \int \frac{dS'}{v_F(S')}d\epsilon'$$

where $dS' \equiv d^2k$ is a surface integral along the surface of constant energy and $v_F(S) = \mathbf{n}\cdot\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}$ is the local Fermi velocity normal to this surface. Making this substitution,

$$\Sigma(\omega) = \frac{1}{\int dS}\int \frac{dS\,dS'}{v'_F}d\epsilon' g^2_{\mathbf{k}-\mathbf{k}'}\left[\frac{1+n_{\mathbf{k}-\mathbf{k}'}-f(\epsilon')}{z-(\epsilon'+\omega_{\mathbf{k}-\mathbf{k}'})} + \frac{n_{\mathbf{k}-\mathbf{k}'}+f(\epsilon')}{z-(\epsilon'-\omega_{\mathbf{k}-\mathbf{k}'})}\right]$$

If we introduce a delta function in the phonon frequency into this expression, using the identity $1 = \int d\nu\delta(\nu - \omega_{\mathbf{q}\lambda})$, then we may rewrite it as follows

$$\begin{aligned}\Sigma(\omega) &= \frac{1}{\int dS}\int d\epsilon' d\nu \int \frac{dS\ dS'}{v'_F} g^2_{\mathbf{k}-\mathbf{k}'}\delta(\nu-\omega_{\mathbf{k}-\mathbf{k}'})\left[\frac{1+n(\nu)-f(\epsilon')}{z-(\epsilon'+\nu)} + \frac{n(\nu)+f(\epsilon')}{z-(\epsilon'-\nu)}\right] \\ &= \int_{-\infty}^{\infty} d\epsilon \int_0^\infty d\nu\alpha^2(\nu)F(\nu)\left[\frac{1+n(\nu)-f(\epsilon')}{z-(\epsilon'+\nu)} + \frac{n(\nu)+f(\epsilon')}{z-(\epsilon'-\nu)}\right]\end{aligned} \tag{9.114}$$

where the function

$$F(\omega) = \sum_{\mathbf{q},\lambda}\delta(\omega-\omega_{\mathbf{q}\lambda})$$

is the phonon density of states, and

$$\alpha^2F(\nu) = \frac{1}{\int dS}\int \frac{dS\ dS'}{v'_F}\delta(\omega-\omega_{\mathbf{k}-\mathbf{k}'})g^2_{\mathbf{k}-\mathbf{k}'\lambda}$$

is the Fermi surface average of the phonon matrix element and density of states. With this definition, we may rewrite the self energy as

$$\boxed{\Sigma(z) = \int_{-\infty}^{\infty} d\epsilon \int_0^\infty d\nu\alpha^2(\nu)F(\nu)\left[\frac{1+n(\nu)-f(\epsilon)}{z-(\epsilon+\nu)} + \frac{n(\nu)+f(\epsilon)}{z-(\epsilon-\nu)}\right],}$$

where the energy dependence of the electron density of states has been neglected. This is a very practical form for the electron self-energy. In practice, most of the energy dependence in α^2F is determined by the phonon density of states. As we shall see later, in a conventional electron-phonon superconductor, one may infer the function α^2F using the density of electron states in the superconductor measured by tunneling in the superconducting state.

9.7.2 Mass Renormalization by the electron phonon interaction

Our simplified expression for of the self-energy enables us to examine how electron propagation is modified by the exchange of virtual phonons. Let us expand the electron-phonon self energy around zero frequency in the ground-state. In the ground-state,

$$\begin{aligned}\Sigma(\omega) &= \int_{-\infty}^{\infty} d\epsilon \int_0^{\infty} d\nu \alpha^2(\nu)F(\nu)\left[\frac{\theta(\epsilon)}{z-(\epsilon+\nu)} + \frac{\theta(-\epsilon)}{z-(\epsilon'-\nu)}\right] \\ &= \int_0^{\infty} d\nu \alpha^2(\nu)F(\nu)\ln\left[\frac{\nu-z}{\nu+z}\right]\end{aligned}$$

so that at low frequencies,

$$\Sigma(\omega) = \Sigma(0) - \lambda\omega$$

where

$$\begin{aligned}\lambda &= -\frac{d\Sigma(\omega)}{d\omega}\Big|_{\omega=0} \\ &= 2\int d\nu \frac{\alpha^2(\nu)F(\nu)}{\nu}\end{aligned} \tag{9.115}$$

If we look at our definition of $\alpha^2 F$, we see that this expression is the Fermi surface average of the electron phonon coupling constant defined in (9.113).

Now at low energies, we can write the electron propagator in terms of the quasiparticle energies, as follows

$$\begin{aligned}\mathcal{G}(\mathbf{k},\omega-i\delta) &= \frac{1}{\omega-\epsilon_{\mathbf{k}}-\Sigma(\omega-i\delta)} \\ &= \frac{1}{\omega-\underbrace{\epsilon_{\mathbf{k}}-\Sigma(\epsilon_k^*-i\delta)}_{\epsilon_{\mathbf{k}}^*-i\Gamma/2}+\lambda(\omega-\epsilon_k^*)},\end{aligned} \tag{9.116}$$

or

$$\boxed{\mathcal{G}(\mathbf{k},\omega-i\delta) = \frac{Z}{\omega-\epsilon_{\mathbf{k}}^*-i\Gamma^*/2}} \tag{9.117}$$

where

$$\begin{aligned} Z &= (1+\lambda)^{-1} && \text{wavefunction renormalization} \\ \epsilon_{\mathbf{k}}^* &= \epsilon_{\mathbf{k}}+\Sigma(\epsilon_k^*) && \text{quasiparticle energy} \\ \Gamma^* &= 2ZIm\Sigma(\epsilon_{\mathbf{k}}^*-i\delta) && \text{quasiparticle decay rate.}\end{aligned} \tag{9.118}$$

We see that in the presence of the electron phonon interaction, electron quasiparticles are still well-defined at low temperatures. Indeed, at the Fermi surface, $\Gamma^* = 0$ in the ground-state, so that electron

quasiparticles are infinitely long-lived. This is an example of a Landau Fermi liquid, discussed in chapter 8. If we differentiate $\epsilon_{\mathbf{k}}$ with respect to $\epsilon_{\mathbf{k}}^*$, we obtain

$$\frac{d\epsilon_{\mathbf{k}}}{d\epsilon_{\mathbf{k}}^*} = (1+\lambda) = \left(\frac{m^*}{m}\right)$$

so that the effective mass of the electron is enhanced by the cloud of virtual phonons which trails behind it. The density of states is also renormalized in the same way

$$N(0)^* = \frac{d\epsilon_{\mathbf{k}}}{d\epsilon_{\mathbf{k}}^*}N(0) = N(0)(1+\lambda)$$

while the electron group velocity is renormalized downwards according to

$$v_F^* = \nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}^* = \frac{d\epsilon_{\mathbf{k}}^*}{d\epsilon_{\mathbf{k}}}\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}} = Zv_F$$

Thus the electron phonon interaction drives up the mass of the electron, effect of squeezing the one-particle states more closely together and driving the electron group velocity downwards. This in turn will mean that the linear coefficient of the electronic specific heat $C_v = \gamma^* T$

$$\gamma^* = \frac{\pi^2 k_B^2}{3}N^*(0) = \gamma_0(1+\lambda)$$

is enhanced.

We can give the wavefunction renormalization another interpretation. Recall that using the method of contour integration, we can always rewrite the Matsubara representation of the Green function

$$G(\mathbf{k},\tau) = T\sum_n G(\mathbf{k},i\omega_n)e^{-i\omega_n\tau}$$

as

$$G(\mathbf{k},\tau) = -\int \frac{d\omega}{\pi}\left[(1-f(\omega))\theta(\tau) - f(\omega)\theta(-\tau)\right]A(\mathbf{k},\omega)e^{-\omega\tau}, \tag{9.119}$$

where $A(\mathbf{k},\omega) = ImG(\mathbf{k},\omega-i\delta)$ is the spectral function. Now, from the normalization of the fermionic commutation relation $\{c_{\mathbf{k}\sigma}, c^\dagger{}_{\mathbf{k}\sigma}\} = 1$, we deduce that the spectral function is normalized:

$$\begin{aligned}1 &= \langle\{c_{\mathbf{k}\sigma}, c^\dagger{}_{\mathbf{k}\sigma}\}\rangle = \overbrace{G(\mathbf{k},0^-)}^{\langle c^\dagger{}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle} - \overbrace{G(\mathbf{k},0^+)}^{-\langle c_{\mathbf{k}\sigma}c^\dagger{}_{\mathbf{k}\sigma}\rangle} \\ &= \int \frac{d\omega}{\pi}A(\mathbf{k},\omega)\end{aligned} \tag{9.120}$$

The quasiparticle part of the spectral function (9.117) is a Lorentzian of width $\Gamma_{\mathbf{k}}^*$, weight πZ, and since the width $\Gamma_{\mathbf{k}}^* \to 0$ as $\epsilon_{\mathbf{k}}^*$ gets closer to the Fermi energy, we deduce that for $k \sim k_F$, the quasiparticle part of the spectral function ever more closely represents a delta function of weight Z, so that

$$\frac{1}{\pi}A(\mathbf{k},\omega) \sim Z\delta(\omega-\epsilon_{\mathbf{k}}^*) + \text{incoherent background}$$

where the incoherent background is required so that the total frequency integral of the spectral function is equal to unity.

Now from (9.119), we see that the ground-state occupancy of the electron momentum state $\mathbf{k}$ is given by

$$\begin{aligned} n_{\mathbf{k}\sigma} &= \langle \hat{n}_{\mathbf{k}\sigma}\rangle_{T=0} = -G(\mathbf{k},0^-) = \int \frac{d\omega}{\pi} f(\omega)A(\mathbf{k},\omega)\Big|_{T=0} \\ &= \int_{-\infty}^{0} \frac{d\omega}{\pi} A(\mathbf{k},\omega), \qquad (T=0) \end{aligned} \tag{9.121}$$

The presence of the quasiparticle pole in the spectral function means that at the Fermi surface, there is a discontinuity in the occupancy given by

$$n_{\mathbf{k}\sigma}|_{k=k_F^-} - n_{\mathbf{k}\sigma}|_{k=k_F^+} = Z = \frac{1}{1+\lambda}$$

as shown in Fig. 9.6

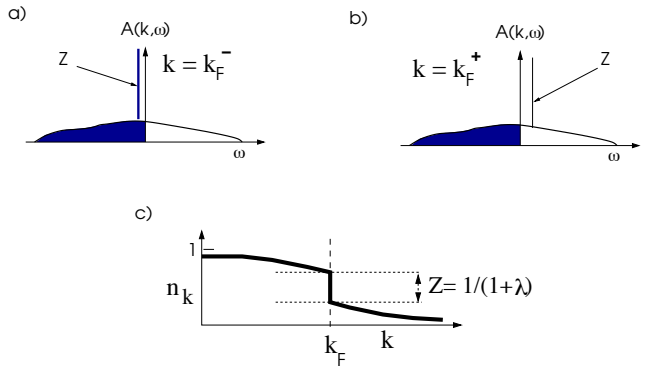


Figure 9.6: Illustrating the relationship between the coherent, quasiparticle component in the electron spectral function, and the discontinuity in the momentum-space occupancy at the Fermi surface due to the electron-phonon interaction. a) Spectral function just below the Fermi surface - quasiparticle peak occupied. b) Spectral function just above Fermi surface - quasiparticle peak unoccupied. c) Momentum space occupancy $n_{\mathbf{k}}$.

Remarks:

- *The survival of a sharp "coherent" delta-function peak in the quasiparticle spectral function, together with this sharp precipace-like discontinuity in the momentum-space occupancy, are one of the hallmark features of the Landau Fermi liquid. In an electron-phonon mediated superconductor, it is the coherent part of the spectral function which condenses into the pair condensate.*

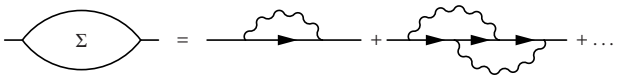
- *At first sight, one might imagine that since the density of states $N^*(0) = (1+\lambda)N(0)$ is enhanced, the magnetic susceptibility will follow suit. In actual fact, the compression of the density of states produced by phonons is always located at the Fermi energy, and this means that if the electron phonon interaction is turned on adiabatically, it does not affect the Fermi momenta of either up, or down electrons, so that the magnetization, and hence the magnetic susceptibility are unaffected by the electron phonon interaction.*

9.7.3 Migdal's theorem.

At first sight, one might worry about the usefulness of our leading order self-energy correction. We have already seen that the size of the electron phonon interaction λ is of order unity. So what permits us to ignore the vertex corrections to the self energy?

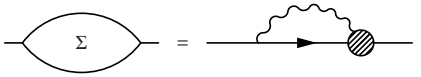
One of the classic early results in the electron phonon problem, is Migdal's theorem[9], according to which that the renormalization of the electron-phonon coupling by phonon exchange, is of order $\sqrt{\frac{m}{M}}$. Migdal's theorem is a result of the huge mismatch between the electron and phonon dispersion. Basically- when an electron scatters off a phonon, it moves away so fast that other phonons can not "catch up" with the outgoing electron.

Migdal's theorem concerns the correction to the electron-phonon vertex. Diagramatically, the electron self-energy can be expanded as follows



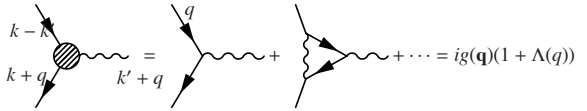
(9.122)

which we can denote by the shorthand



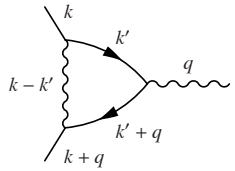
(9.123)

Here, the shaded circle denotes the vertex part, given by



(9.124)

We shall discuss the leading order vertex correction,



$$= (ig_{\mathbf{q}})\Lambda(q) \tag{9.125}$$

where the vertex function $\Lambda(q)$ is given by

$$\Lambda(q) = T\sum_{k'\equiv(i\omega'_n,\mathbf{k}')}(ig_{\mathbf{k}-\mathbf{k}'})^2 G(k'+q)G(k')D(k-k') \tag{9.126}$$

We are interested in an order of magnitude estimate of this quantity.

Now at low temperatures, we can replace the summation over the Matsubara frequency can be replaced by an integral,

$$T\sum_{\omega'_n} \to \int \frac{d\omega'_n}{2\pi}$$

so that

$$\Lambda(q) = -\int\frac{d\omega'_n}{2\pi}\int\frac{d^3k'}{(2\pi)^3}(g_{\mathbf{k}-\mathbf{k}'})^2 G(k'+q)G(k')D(k-k')$$

Now the propogator

$$D(k-k') = -\frac{\omega_{\mathbf{k}-\mathbf{k}'}}{(\omega_n-\omega'_n)^2+\omega^2_{\mathbf{q}}}$$

vanishes as $1/(\omega'_n)^2$ in the region where $|\omega_n - \omega'_n| \gtrsim \omega_D$, so we restrict this integral, writing

$$\Lambda(q) = -\int_{-\omega_D}^{\omega_D}\frac{d\omega'_n}{2\pi}\int\frac{d^3k'}{(2\pi)^3}(g_{\mathbf{k}-\mathbf{k}'})^2 D(k-k')G(k'+q)G(k')$$

Inside the restricted frequency integral, to obtain an estimate of this quantity, we shall replace $g^2_{\mathbf{k}-\mathbf{k}'}D(\mathbf{k}-\mathbf{k}') \sim a^3 g \times 2\omega_{\mathbf{k}-\mathbf{k}'}D(\mathbf{k}-\mathbf{k}') \sim -g$, since $2\omega_{\mathbf{k}-\mathbf{k}'}D(\mathbf{k}-\mathbf{k}') \sim -1$. To good approximation, the frequency integral may be replaced by a single factor ω_D, so that

$$\Lambda(q) \sim \omega_D g a^3 \overbrace{\int\frac{d^3k'}{(2\pi)^3}G(k'+q)G(k')\Big|_{\omega'_n=\omega_n}}^{\sim\frac{(k_Fa)^3}{\epsilon_F^2}}.$$

Now inside the momentum summation over $\mathbf{k}'$, the electron momenta are unrestricted so the energies $\epsilon_{\mathbf{k}'}$ and $\epsilon_{\mathbf{k}'+\mathbf{q}}$ are far from the Fermi energy and we may estimate this term as of order $\frac{(k_Fa)^3}{\epsilon_F^2}$. Putting these results together,

$$\Lambda \sim g\omega_D\frac{(k_Fa)^3}{\epsilon_F^2}$$

Now since $g \sim \lambda\epsilon_F$ and $(k_Fa)^3 \sim 1$, we see that

$$\Lambda \sim \lambda\frac{\omega_D}{\epsilon_F} \sim \sqrt{\frac{m}{M}}$$

In otherwords, even though the electron phonon interaction is of order unity, the large ratio of electron to ion mass leads to a very small vertex correction.
Remarks:

- *Perhaps the main difficulty of the Migdal argument, is that it provides a false sense of security to the theorist- giving the impression that one has "proven" that the perturbative treatment of the electron phonon interaction is always justified. Migdal's argument is basically a dimensional analysis. The weak-point of the derivation, is that the dimensional analysis does not work for those scattering events where the energies of the scattered electrons are degenerate. While such scattering events may make up a small contribution to the overall phase space contributing to the self-energy, they become important because the associated scattering amplitudes can develop strong singularities that ultimately result in a catastrophic instability of the Fermi liquid. The dimensional analysis in the Migdal argument breaks down when electrons inside the loop have almost degenerate energies. For example, the Migdal calculation, does not work for the case where* $\mathbf{q}$ *is close to a nesting vector of the Fermi surface, when* $\mathbf{q}$ *spans two nested Fermi surfaces, this causes* $\epsilon_{\mathbf{k}'}$ *and* $\epsilon_{\mathbf{k}'+\mathbf{q}}$ *to become degenerate, enhancing the size of the vertex by a factor of* $\epsilon_F/\omega_D \times \log(\omega_D/T)$*. The singular term ultimately grows to a point where an instability to a density wave takes place, producing a charge density wave. The other parallel instability is the Cooper instability, which is a singular correction to the particle-particle scattering vertex, caused by the degeneracy of electron energies for electrons of opposite momenta.*

9.8 Appendix A

In this appendix, we consider the Hamiltonian

$$H = \overbrace{\sum_\lambda \epsilon_\lambda \psi^\dagger{}_\lambda\psi_\lambda}^{H_0} - \overbrace{\sum_\lambda\left[\bar{z}_\lambda(\tau)\psi_\lambda + \psi^\dagger{}_\lambda\right)_\lambda\Big]}^{-V_I}$$

and show that the generating functional

$$\begin{aligned} Z_0[\bar\eta,\eta] &= Z_0\langle T e^{-\int_0^\beta V_I(\tau)d\tau}\rangle_0 \\ &= Z_0\langle T\exp\left[\int_0^\beta d\tau\sum_\lambda\left(\bar\eta_\lambda(\tau)\psi_\lambda(\tau) + \psi^\dagger{}_\lambda(\tau)\eta_\lambda(\tau)\right)\right]\rangle_0 \end{aligned} \tag{9.127}$$

is explicitly given by

$$\begin{aligned}\frac{Z_0[\bar\eta,\eta]}{Z_0} &= \exp\left[-\sum_\lambda \int_0^\beta d\tau_1 d\tau_2 \bar\eta_\lambda(1) G_\lambda(\tau_1-\tau_2)\eta_\lambda(2)\right]\\ G_\lambda(\tau_1-\tau_2) &= -\langle T\psi_\lambda(\tau_1)\psi^\dagger{}_\lambda(\tau_2)\rangle \end{aligned} \tag{9.128}$$

for both bosons and fermions.

We begin by evaluating the equation of motion of the fields in the Heisenberg representation:

$$\frac{\partial\psi_\lambda}{\partial\tau} = [H,\psi_\lambda] = -\epsilon_\lambda\psi_\lambda(\tau) + \eta_\lambda(\tau)$$

Multiplying this expression by the integrating factor $e^{\epsilon_\lambda\tau}$, we obtain

$$\frac{\partial}{\partial\tau}\left[e^{\epsilon_\lambda\tau}\psi_\lambda(\tau)\right] = e^{\epsilon_\lambda\tau}\eta_\lambda(\tau)$$

which we may integrate from $\tau' = 0$ to $\tau' = \tau$, to obtain

$$\psi_\lambda(\tau) = e^{-\epsilon_\lambda\tau}\psi_\lambda(0) + \int_0^\tau d\tau' e^{-\epsilon_\lambda(\tau-\tau')}\eta_\lambda(\tau')d\tau'$$

We shall now take expectation values of this equation, so that

$$\langle\psi_\lambda(\tau)\rangle = e^{-\epsilon_\lambda\tau}\langle\psi_\lambda(0)\rangle + \int_0^\tau d\tau' e^{-\epsilon_\lambda(\tau-\tau')}\eta_\lambda(\tau')d\tau' \tag{9.129}$$

If we impose the boundary condition $\langle\psi_\lambda(\beta)\rangle = \zeta\langle\psi_\lambda(0)\rangle$, where $\zeta = 1$ for bosons and $\zeta = -1$ for fermions, then we deduce that

$$\langle\psi_\lambda(0)\rangle = \zeta n_\lambda \int_0^\beta e^{\epsilon_\lambda\tau'}\eta_\lambda(\tau')d\tau',$$

where $n_\lambda = 1/(e^{\beta\epsilon_\lambda} - \zeta)$ is the Bose ($\zeta = 1$), or Fermi function $\zeta = -1$. Inserting this into (9.129), we obtain

$$\langle\psi_\lambda(\tau)\rangle = \zeta n_\lambda \int_0^\beta e^{-\epsilon_\lambda(\tau-\tau')}\eta_\lambda(\tau')d\tau' + \int_0^\beta e^{-\epsilon_\lambda(\tau-\tau')}\theta(\tau-\tau')\eta_\lambda(\tau')d\tau', \tag{9.130}$$

where we have introduced a theta function in the second term, in order to extend the upper limit of integration to β. Rearranging this expression, we obtain

$$\begin{aligned}\langle\psi_\lambda(\tau)\rangle &= \int_0^\beta d\tau' \overbrace{e^{-\epsilon_\lambda}(\tau-\tau')\left[(1+\zeta n_\lambda)\theta(\tau-\tau') + \zeta n_\lambda\theta(\tau'-\tau)\right]}^{-\mathcal{G}_\lambda(\tau-\tau')}\\ &= -\int_0^\beta d\tau'\mathcal{G}_\lambda(\tau-\tau')\eta_\lambda(\tau')\end{aligned} \tag{9.131}$$

so $\mathcal{G}_\lambda(\tau)$ is the imaginary time response of the field to the source term. We may repeat the same procedure for the expectation value of the creation operator. The results of these two calculations may be summarized as

$$\begin{aligned}\langle\psi_\lambda(\tau)\rangle &= \frac{\delta Z[\bar\eta,\eta]}{\delta\bar\eta(\tau)} = -\int_0^\beta d\tau'\mathcal{G}_\lambda(\tau-\tau')\eta_\lambda(\tau')\\ \langle\psi^\dagger{}_\lambda(\tau)\rangle &= \frac{\delta Z[\bar\eta,\eta]}{\delta\eta(\tau)} = -\int_0^\beta d\tau'\bar\eta(\tau)\mathcal{G}_\lambda(\tau-\tau').\end{aligned} \tag{9.132}$$

Notice how the creation field propagates backwards in time from the source. The common integral to these two expression is

$$\ln Z[\bar\eta,\eta] = \ln Z_0 - \int_0^\beta d\tau d\tau'\bar\eta_\lambda(\tau)G_\lambda(\tau-\tau')\eta_\lambda(\tau')$$

where the constant term $\ln Z_0$ has to be intependent of both η and $\bar\eta$. The exponential of this expression recovers the result (9.128).

9.9 Exercises

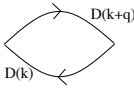
1. Use the method of complex contour integration to carry out the Matsubara sums in the following:

   (i) Derive the density of a spinless Bose Gas at finite temperature from the boson propagator $D(k) \equiv D(\mathbf{k}, i\nu_\mathbf{n}) = [i\nu_\mathbf{n} - \omega_\mathbf{k}]^{-1}$, where $\omega_\mathbf{k} = E_\mathbf{k} - \mu$ is the energy of a boson, measured relative to the chemical potential.

   $$\rho(T) = \frac{N}{V} = V^{-1}\sum_\mathbf{k}\langle T b_\mathbf{k}(0^-)b^\dagger_\mathbf{k}(0)\rangle = -(\beta V)^{-1}\sum_{i\nu_n,\mathbf{k}} D(k)e^{i\nu_n 0^+}. \tag{9.133}$$

   How do you need to modify your answer to take account of Bose Einstein condensation?

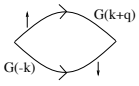
   (ii) The dynamic charge-susceptibility of a free Bose gas, i.e

   $\chi_c(q,i\nu_n) =$ 

   $= T\sum_{i\nu_n}\int\frac{d^3k}{(2\pi)^3}D(q+k)D(k).$ (9.134)

   Please analytically extend your final answer to real frequencies.

   (iii) The "pair-susceptibility" of a spin-1/2 free Fermi gas, i.e.

   $\chi_P(q,i\nu_n) =$ 

   $= T\sum_{i\omega_r}\int\frac{d^3k}{(2\pi)^3}G(q+k)G(-k)$ (9.135)

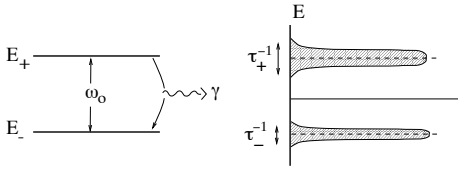
   where $G(k) \equiv G(\mathbf{k}, i\omega_\mathbf{n}) = [i\omega_\mathbf{n} - \epsilon_\mathbf{k}]^{-1}$. (Note the direction of the arrows: why is there no minus sign for the Fermion loop?) Show that the static pair susceptibility, $\chi_P(0)$is given by

   $$\chi_P = \int\frac{d^3k}{(2\pi)^3}\frac{\tanh[\beta\epsilon_\mathbf{k}/2]}{2\epsilon_\mathbf{k}} \tag{9.136}$$

   Can you see that this quantity diverges at low temperatures? How does it diverge, and why ?

2. A simple model an atom with two atomic levels coupled to a radiation field is described by the Hamiltonian

$$H = H_o + H_I + H_{\rm photon}, \tag{9.137}$$



where

$$H_o = \bar{E}_- c^\dagger_- c_- + \bar{E}_+ c^\dagger_+ c_+ \tag{9.138}$$

describes the atom, treating it as a *fermion*

$$H_I = V^{-1/2} \sum_{\vec{q}} g(\omega_{\vec{q}}) \Big(c^\dagger_+ c_- + c^\dagger_- c_+ \Big) \Big[a^\dagger_{\vec{q}} + a_{-\vec{q}} \Big] \tag{9.139}$$

describes the coupling to the radiation field (V is the volume of the box enclosing the radiation) and

$$H_{photon} = \sum_{\vec{q}} \omega_{\vec{q}} a^\dagger_{\vec{q}} a_{\vec{q}}, \qquad (\omega_q = cq) \tag{9.140}$$

is the Hamiltonian for the electromagnetic field. The "dipole" matrix element $g(\omega)$ is weak enough to be treated by second order perturbation theory and the polarization of the photon is ignored.

(i) Calculate the self-energy $\Sigma_+(\omega)$ and $\Sigma_-(\omega)$ for an atom in the + and − states.

(ii) Use the self-energy obtained above to calculate the life-times $\tau_\pm$ of the atomic states, i.e.

$$\tau^{-1}_\pm = 2{\rm Im}\Sigma_\pm(\bar{E}_\pm - i\delta). \tag{9.141}$$

If the gas of atoms is non-degenerate, i.e the Fermi functions are all small compared with unity, $f(E_\pm) \sim 0$ show that

$$\begin{aligned} \tau^{-1}_+ &= 2\pi |g(\omega_o)|^2 F(\omega_o)[1 + n(\omega_o)] \\ \tau^{-1}_- &= 2\pi |g(\omega_o)|^2 F(\omega_o) n(\omega_o), \end{aligned} \tag{9.142}$$

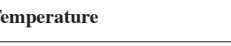
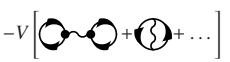
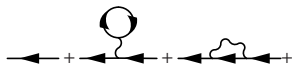
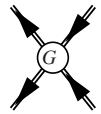
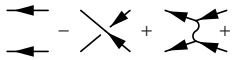
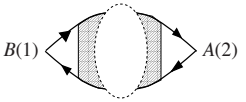
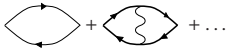
where $\omega_o = \bar{E}_+ - \bar{E}_-$ is the separation of the atomic levels and

$$F(\omega) = \int \frac{d^3q}{(2\pi)^3} \delta(\omega - \omega_q) = \frac{\omega^2}{2\pi c^3} \tag{9.143}$$

is the density of state of the photons at energy ω. What do these results have to do with stimulated emission? Do your final results depend on the initial assumption that the atoms were fermions?

(iii)Why is the decay rate of the upper state larger than the decay rate of the lower state by the factor $[1 + n(\omega_0)]/n(\omega_0)$?

Table. 10.3 Relationship With Physical Quantities: Finite Temperature

ΔF	$-V \sum\{\text{linked clusters}\}$	
$\ln Z/Z_o$	$V\beta \sum\{\text{linked clusters}\}$	
 $-\langle T\psi(2)\psi^\dagger(1)\rangle$	$\sum\{\text{Two leg diagrams}\}$	
$(-1)^n\langle T\psi(1)\ldots\psi^\dagger(2n)\rangle$  $n = 2$	$\sum\{\text{2n- leg diagrams}\}$	
Response Functions $\langle\psi\|T[A(2)B(1)]\|\psi\rangle = \chi^T_{AB}$  $i\langle[A(2),B(1)]\rangle\theta(t_1 - t_2) = \chi_{AB}$	$\chi_{AB} = \chi^T_{AB}(\omega - i\delta)$	

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Chapter 10

Fluctuation Dissipation Theorem and Linear Response Theory

10.1 Introduction

In this chapter we will discuss the deep link between fluctuations about equilibrium, and the response of a system to external forces. If the susceptibility of a system to external change is large, then the fluctuations about equilibrium are expected to be large. The mathematical relationship that quantifies this this connection is called the "fluctuation-dissipation" theorem. We shall discuss and derive this relationship in this chapter. It turns out that the link between fluctuations and dissipation also extends to imaginary time, enabling us to relate equilibrium correlation functions and response functions to the imaginary time Greens function of the corresponding variables.

To describe the fluctuations and response at a finite temperature we will introduce three related three types of Green function- the correlation function $S(t)$,

$$S(t-t') = \langle A(t)\, A(t')\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} S(\omega),$$

the dynamical susceptibility $\chi(t)$

$$\chi(t-t') = i\langle [A(t), A(t')]\rangle \theta(t-t'),$$

which determines the retarded response

$$\langle A(t)\rangle = \int_{-\infty}^{\infty} dt' \chi(t-t') f(t'), \quad \langle A(\omega)\rangle = \chi(\omega) f(\omega),$$

to a force $f(t)$ term coupled to A inside the Hamiltonian $H_I = -f(t)A(t)$, and lastly, the imaginary time response function $\chi(\tau)$

$$\chi(\tau - \tau') = \langle T A(\tau) A(\tau')\rangle$$

.

The fluctuation dissipation theorem relates the Fourier transforms of these quantities. according to

$$\underbrace{S(\omega)}_{\text{Fluctuations}} = 2\hbar[\overbrace{1}^{\text{Quantum}} + \overbrace{n_B(\omega)}^{\text{Thermal}}] \underbrace{\chi''(\omega)}_{\text{Dissipation}},$$

where $\chi''(\omega) = \text{Im}\,\chi(\omega)$ describes the dissipative part of the response function. In the limit, $\omega << k_B T$, when $n(\omega) \sim k_B T/\hbar\omega$, this result reverts to the classical fluctuation-dissipation theorem,

$$S(\omega) = \frac{2k_B T}{\omega}\chi''(\omega).$$

Thus in principle, if we know the correlation functions in thermal equilibrium, we can compute the response function of the system.

The dissipative response of the system also enters into the Kramer's Kronig expansion of the response function,

$$\chi(z) = \int \frac{d\omega}{\pi} \frac{1}{\omega - z}\chi''(\omega)$$

and this expression can be used to analytically extend $\chi(\omega)$ into the complex plane. In practice, the theorist takes advantage of a completely parallel fluctuation-dissipation theorem which exists in imaginary time. The imaginary time correlation function $\chi(\tau)$ is periodic in time. $\chi(\tau+\beta) = \chi(\tau)$, and has an discrete Matsubara Fourier expansion, given by

$$\chi(\tau) = \langle T A(\tau) A(0)\rangle = \frac{1}{\beta}\sum_n e^{-i\nu_n \tau}\chi_M(i\nu_n)$$

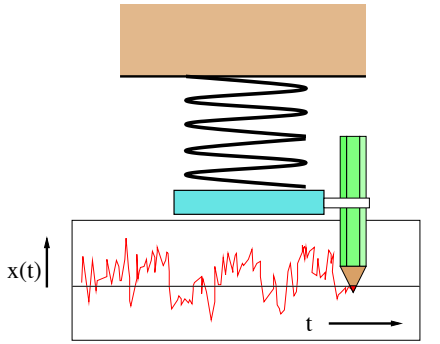
The key relation between this function and the physical response function is that

$$\chi_M(i\nu_n) = \chi(z).|_{z=i\nu_n}.$$

This relation permits us to compute the physical response function by analytically continuing the Fourier components of the imaginary-time correlation functions onto the real axis.

To understand these relations, we need first to understand the nature of the quantum mechanical response functions. We shall then carry out a "spectral decomposition" of each of the above functions, deriving the fluctuation dissipation theorem by showing that the same underlying matrix elements enter into each expression. A heuristic understanding of the relationship between fluctuations and dissipation, is obtained by examining a classical example. The main difference between the classical and the quantum fluctuation-dissipation theorem, is that in classical mechanics we are obliged to explicitly include the external sources of noise, whereas in the quantum case, the noise is intrinsic, and we can analyse the fluctuations without any specific reference to external sources of noise. Nevertheless, the classical case is highly pedagogical, and it is this limit that we shall consider first.

10.2 Fluctuation dissipation theorem for a classical harmonic oscillator



$$\overbrace{\langle x(t)x(0)\rangle}^{fluctuations} = 2k_BT\int\frac{d\omega}{2\pi}\underbrace{\frac{\chi''(\omega)}{\omega}}_{dissipation}e^{-i\omega t}$$

Figure 10.1: Fluctuations in a classical harmonic oscillator are directly related to the dissipative response function via the "fluctuation dissipation theorem".

In a classical system, to examine correlation functions we need to include an explicit source of external noise. To illustrate the procedure, consider a harmonic oscillator in thermal equilibrium inside a viscous medium. Suppose that thermal fluctuations give rise to a random force, acting on the oscillator, according to the quation of motion:

$$m(\ddot{x} + \omega_o^2 x) + \eta\dot{x} = f(t)$$

If we Fourier transform this relationship, we obtain

$$\begin{aligned} x(\omega) &= \chi(\omega)f(\omega) \\ \chi(\omega) &= [m(\omega_0^2 - \omega^2) - i\omega\eta]^{-1} \end{aligned} \qquad (10.1)$$

Here $\chi(\omega)$ is the response function , or susceptibility to the external force. The imaginary part of

the susceptibility governs the dissipation and is given by

$$\chi''(\omega) = \frac{\omega\eta}{m(\omega_0^2 - \omega^2) + \omega^2\eta^2} = |\chi(\omega)|^2\omega\eta. \qquad (10.2)$$

Now let us consider the fluctuations in thermal equilibrium. Over long time periods, we expect the two-point correlation function to be purely a function of the time difference:

$$\langle x(t)x(t')\rangle = \langle x(t-t')x(0)\rangle$$

The power spectrum of fluctuations is defined as

$$\langle|x(\omega)|^2\rangle = \int dt\langle x(t)x(0)\rangle e^{i\omega t}$$

and the inverse relation gives

$$\langle x(t)x(t')\rangle = \int\frac{d\omega}{2\pi}e^{-i\omega(t-t')}\langle|x(\omega)|^2\rangle.$$

Now in thermal equilibrium, the equipartition theorem tells us that

$$\frac{m\omega_0^2}{2}\langle x^2\rangle = \frac{k_BT}{2},$$

or

$$\langle x^2\rangle = \int\frac{d\omega}{2\pi}\langle|x(\omega)|^2\rangle = \int\frac{d\omega}{2\pi}|\chi(\omega)|^2\langle|f(\omega)|^2\rangle = \frac{k_BT}{m\omega_0^2}$$

Since the integrand is very sharply peaked around $|\omega| = \omega_0$, we replace $\langle|f(\omega)|^2\rangle \to \langle|f(\omega_0)|^2\rangle$ in the above expression. Replacing $|\chi(\omega)|^2 \to \frac{1}{\omega\eta}\chi''(\omega)$ we then obtain

$$\frac{k_BT}{m\omega_0^2} = \frac{\langle|f(\omega_0)|^2\rangle}{2\eta}\int\frac{d\omega}{\pi}\frac{\chi''(\omega)}{\omega} = \frac{|f(\omega_0)|^2}{2\eta m\omega_0^2}.$$

so that the spectrum of force fluctuations is determined by the viscosity η

$$\langle|f(\omega_0)|^2\rangle = 2\eta k_BT.$$

Now if we assume that the noise spectrum it depends only on the properties of the viscous medium in which the oscillator is embedded, and that it does not depend on the properties of the oscillator, then we expect this expression holds for any frequency ω_0, and since it is *independent* of the frequency, we conclude that the power spectrum of the force is a flat function of frequency, enabling us to replace $\omega_0 \to \omega$ in the above expression. This implies that in thermal equilibrium, the force coupling the system to the environment is a source of white noise of amplitude which depends on the viscosity of the medium

$$\langle f(t)f(t')\rangle = \int\frac{d\omega}{2\pi}e^{-i\omega(t-t')}\overbrace{\langle|f(\omega)|^2\rangle}^{2\eta k_BT} = 2\eta k_BT\delta(t-t')$$

We can now compute the noise spectrum of fluctuations, which is given by

$$S(\omega) = \langle |x(\omega)|^2 \rangle = |\chi(\omega)|^2 \langle |f(\omega)|^2 \rangle = \langle |f(\omega)|^2 \rangle \frac{\chi''(\omega)}{\omega\eta} = \frac{2k_BT}{\omega}\chi''(\omega).$$

This expression relates the thermal fluctuations of a classical system to the dissipation, as described by the imaginary part of the response function, $\chi''(\omega)$.

10.3 Quantum Mechanical Response Functions.

Suppose we couple a force f to variable A. For later generality, it suits our need to consider a force in both in real and imaginary time, with Hamiltonian

$$\begin{aligned} H &= H_o - f(t)A \\ H &= H_o - f(\tau)A. \end{aligned} \tag{10.3}$$

We shall now show that the response to these forces are given by

$$\begin{aligned} \langle A(t)\rangle &= \langle A\rangle + \int_{-\infty}^{\infty} \chi(t-t')f(t')dt' \\ \langle A(\tau)\rangle &= \langle A\rangle + \int_0^{\beta} \tilde{\chi}(\tau-\tau')f(\tau')d\tau' \end{aligned} \tag{10.4}$$

$$\begin{aligned} \chi(t-t') &= i\langle [A(t),\ A(t')]\rangle\theta(t-t') \\ \tilde{\chi}(\tau-\tau') &= \langle TA(\tau)A(\tau')]\rangle - \langle A\rangle^2 \end{aligned} \tag{10.5}$$

where $\langle A\rangle$ is the value of A in thermal equilibrium. Let us begin in real time. Using the interaction representation, we know that

$$A_H(t) = U^\dagger(t)A_I(t)\ U(t),$$

where

$$U(t) = T\exp i\int_{-\infty}^{t} dt' A_I(t')f(t').$$

Remembering that the interaction representation corresponds to the Heisenberg representation for

H_o, we can drop the subscript on $A_I(t) \equiv A(t)$, so that to linear order in $f(t)$,

$$\begin{aligned} U(t) &= 1 + i\int_{-\infty}^{t} dt' A(t')f(t'), \\ U^\dagger(t) &= 1 - i\int_{-\infty}^{t} dt' A(t')f(t') \end{aligned}$$

so that

$$A_H(t) = A(t) + i\int_{-\infty}^{t} dt' [A(t), A(t')]\, f(t'),$$

In thermal equilibrium if $\langle A(t)\rangle = \langle A\rangle$, so the response to the applied force is given by

$$\langle A_H(t)\rangle = \langle A\rangle + \int_{-\infty}^{+\infty} dt'\ \chi(t-t')\, f(t'),$$

where

$$\chi(t-t') = i\langle [A(t), A(t')]\,\rangle\theta(t-t')$$

is the "retarded response function", also known as the "dynamical susceptibility". The above equation is particularly interesting, for it relates a quantum-mechanical response function to a correlation-function.

Let us now consider imaginary time. In this case, the partition function in the presence of the perturbation is

$$Z = Z_0\langle T\exp\int_0^{\beta} d\tau f(\tau)A_I(\tau)\rangle_0$$

The expectation value of $A(\tau)$ is then given by

$$\begin{aligned} \langle A(\tau)\rangle &= \frac{\delta \ln Z}{\delta f(\tau)} = \frac{\langle TA(\tau)\exp\int_0^{\beta} d\tau' f(\tau')A_I(\tau')\rangle}{\langle T\exp\int_0^{\beta} d\tau' f(\tau')A_I(\tau')\rangle} \\ &= \langle A\rangle + \int_0^{\beta} d\tau' \overbrace{\left[\langle TA(\tau)A(\tau')\rangle - \langle A\rangle^2\right]}^{\tilde{\chi}(\tau-\tau')} f(\tau') + O(f^2) \end{aligned} \tag{10.6}$$

so that

$$\begin{aligned} \tilde{\chi}(\tau) &= \langle TA(\tau)A(0)\rangle - \langle A\rangle^2 \\ &= \langle T(A(\tau)-\langle A\rangle)(A(0)-\langle A\rangle)\rangle \end{aligned} \tag{10.7}$$

where the expectation values are to be taken in thermal equilibrium for H_0.

10.4 Fluctuations and Dissipation in a quantum world

Unlike classical mechanics, the quantum Boltzmann formulation of many body physics is naturally tailored to a discussion of the statistics of fluctuations and dissipation. Quantum systems are naturally noisy, and there is no need for us to add any additional noise source to examine the deep link between flucutations and dissipation in a quantum many body system. Indeed, the quantum fluctuation dissipation theorem can be derived in rather mechanistic fashion by carrying out out a spectral decomposition of the various response and correlation functions. The procedure is formally more direct that its classical analogue, but the algebra tends to hide the fact that the underlying physics holds precisely the same link between fluctuations- now both thermal and quantum in character- and dissipation.

To derive the quantum fluctuation theorem, we must first spectrally decompose the correlation function $S(t-t')$ and the response function $\chi(t-t')$.

10.4.1 Spectral decomposition I: the correlation function $S(t-t')$

This is the easiest decomposition of the three to carry out. We begin by expanding the response function in terms of a complete set of energy eigenstates which satisfy

$$\begin{aligned} H|\lambda\rangle &= E_\lambda|\lambda\rangle, \\ \sum_\lambda |\lambda\rangle\langle\lambda| &= 1, \\ \langle\lambda|A(t)|\zeta\rangle &= \left\langle\lambda\left|e^{iHt}Ae^{-iHt}\right|\zeta\right\rangle = e^{-i(E_\zeta-E_\lambda)(t-t')}\langle\lambda|A|\zeta\rangle. \end{aligned}$$

Using these key results, we make the expansion as follows,

$$\begin{aligned} S(t-t') &= \langle A(t)A(t')\rangle \\ &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}\langle\lambda|A(t)|\zeta\rangle\left\langle\zeta\left|A(t')\right|\lambda\right\rangle \\ &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}|\langle\zeta|A|\lambda\rangle|^2 e^{-i(E_\zeta-E_\lambda)(t-t')} \end{aligned} \tag{10.8}$$

If we now Fourier transform this expression, the frequency dependent correlation function can be written

$$\begin{aligned} S(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t}S(t) \\ &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}|\langle\zeta|A|\lambda\rangle|^2 2\pi\delta(E_\zeta-E_\lambda-\omega). \end{aligned} \tag{10.9}$$

This is the frequency spectrum of the correlations.

10.4.2 Spectral decomposition II: the response function $\chi(t-t')$

We now use the same spectral decomposition approach for the response function. In this case, we need to take care of two operator orderings inside the commutator, which yield

$$\begin{aligned} \chi(t-t') &= i\sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}\left\{\langle\lambda|A(t)|\zeta\rangle\left\langle\zeta\left|A(t')\right|\lambda\right\rangle - \left\langle\lambda\left|A(t')\right|\zeta\right\rangle\langle\zeta|A(t)|\lambda\rangle\right\}\theta(t-t') \\ &= i\sum_{\lambda,\zeta} e^{\beta F}(e^{-\beta E_\lambda}-e^{-\beta E_\zeta})|\langle\zeta|A|\lambda\rangle|^2 e^{-i(E_\zeta-E_\lambda)(t-t')}\theta(t-t'). \end{aligned}$$

By introducing the spectral function

$$\chi''(\omega) = \pi(1-e^{-\beta\omega})\sum_{\lambda,\zeta}|\langle\zeta|A|\lambda\rangle|^2\,\delta[\omega-(E_\zeta-E_\lambda)]e^{-\beta(E_\lambda-F)}, \tag{10.10}$$

we see that the retarded response function can be written,

$$\chi(t) = i\int d\omega\, e^{-i\omega t}\theta(t)\chi''(\omega). \tag{10.11}$$

Fourier transforming this result, using

$$i\int_0^\infty dt e^{i(\omega-\omega'+i\delta)t} = \frac{1}{\omega'-\omega-i\delta},$$

we obtain

$$\chi(\omega) = \int\frac{d\omega'}{\pi}\frac{1}{\omega'-\omega-i\delta}\chi''(\omega'). \tag{10.12}$$

This "Kramers-Krönig" relation can be used to extend the response function into the complex plane. Notice that because the response function is *retarded*, $\chi(\omega)$ is analytic in the upper-half complex plane and the poles lie just below the real axis, at $z=\omega'-i\delta$. Finally, taking the imaginary part of this expression, using the Dirac relation $Im[1/(\omega'-\omega-i\delta) = \pi\delta(\omega'-\omega)$, we are able to identify

$$\chi''(\omega) = Im\chi(\omega+i\delta)$$

as the dissipative part of the response function.

10.4.3 Quantum Fluctuation dissipation Theorem

If we compare the relations (10.10) and (10.9), we see that

$$S(\omega) = \frac{2}{1-e^{-\beta\omega}}\chi''(\omega).$$

If we restore $\hbar$, this becomes

$$S(\omega) = \frac{2\hbar}{1-e^{-\beta\hbar\omega}}\chi''(\omega) = 2\hbar\,[1+n_B(\hbar\omega)]\,\chi''(\omega). \tag{10.13}$$

Thus, by carrying out a spectral analysis, we have been able to directly link the correlation function $S(\omega)$ with the dissipative part of the response function $\chi(\omega)$.

10.4.4 Spectral decomposition III: fluctuations in imaginary time

For the final of our three decompositions, we move to imaginary time, and write, $\tau - \tau' > 0$,

$$\begin{aligned}\chi(\tau-\tau') &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda - F)}\left\{\langle\lambda|A(\tau)|\zeta\rangle\left\langle\zeta\left|A(\tau')\right|\lambda\right\rangle\right\} \\ &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}e^{-(E_\lambda-E_\zeta)(\tau-\tau')}|\langle\zeta|A|\lambda\rangle|^2\,.\end{aligned}$$

Now

$$\int_0^\beta d\tau\, e^{i\nu_n\tau}e^{-(E_\lambda-E_\zeta)\tau} = \frac{1}{(E_\zeta - E_\lambda - i\nu_n)}(1-e^{-(E_\lambda-E_\zeta)\beta}),$$

so

$$\begin{aligned}\chi(i\nu_n) &= \int_0^\beta d\tau\, e^{i\nu_n\tau}\chi(\tau) \\ &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}(1-e^{-\beta(E_\zeta-E_\lambda)})\,|\langle\zeta|A|\lambda\rangle|^2\,\frac{1}{(E_\zeta-E_\lambda-i\nu_n)}.\end{aligned}$$

Using (10.10), we can write this as

$$\chi(i\nu_n) = \int \frac{d\omega}{\pi}\frac{1}{\omega - i\nu_n}\chi''(\omega) \tag{10.14}$$

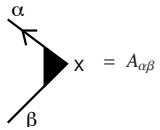
so that $\chi(i\nu_n)$ is the unique analytic extension of $\chi(\omega)$ into the complex plane. Our procedure to calculate response functions will be to write $\chi(i\nu_n)$ in the form 10.14, and to use this to read off $\chi''(\omega)$.

10.5 Calculation of response functions

Having made the link between the imaginary time, and real time response functions, we are ready to discuss how we can calculate response functions from Feynman diagrams. Our procedure is to compute the imaginary time response function, and then analytically continue to real frequencies. Suppose we are interested in the response function for A where,

$$A(x) = \psi^\dagger{}_\alpha(x)A_{\alpha\beta}\psi_\beta(x).$$

(See table 10.0). The corresponding operator generates the vertex



$$= A_{\alpha\beta} \tag{10.15}$$

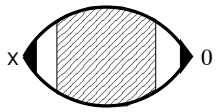
Table. 10.0 Selected Operators and corresponding response function.

Quantity	Operator $\hat{A}$	$A(\mathbf{k})$	Response Function
Density	$\hat{\rho}(x) = \psi^\dagger(x)\psi(x)$	$\rho_{\alpha\beta} = \delta_{\alpha\beta}$	Charge susceptibility
Spin density	$\vec{S}(x) = \psi_\alpha{}^\dagger(x)\left(\frac{\vec{\sigma}}{2}\right)_{\alpha\beta}\psi_\beta(x)$	$\vec{M}_{\alpha\beta} = \mu_B\vec{\sigma}_{\alpha\beta}$	Spin susceptibility
Current density	$\frac{e}{m}\psi^\dagger(x)\left(-i\hbar\overleftrightarrow{\nabla} - e\vec{A}\right)\psi(x)$	$\vec{j} = e\vec{v}_{\mathbf{k}} = e\vec{\nabla}\epsilon_{\mathbf{k}}$	Conductivity
Thermal current	$\frac{\hbar^2}{2m}\psi^\dagger(x)\overleftrightarrow{\nabla}\overleftrightarrow{\partial}_t\psi(x)$	$\vec{j}_T = i\omega_n\vec{v}_{\mathbf{k}} = i\omega_n\vec{\nabla}\epsilon_{\mathbf{k}}$	Thermal conductivity

(Where $\overleftrightarrow{\nabla} \equiv \frac{1}{2}\left(\overrightarrow{\nabla} - \overleftarrow{\nabla}\right)$, $\overleftrightarrow{\partial}_t \equiv \frac{1}{2}\left(\overrightarrow{\partial}_t - \overleftarrow{\partial}_t\right)$)

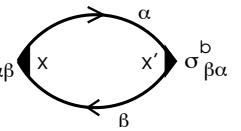
where the spin variables $\alpha\beta$ are to be contracted with the internal spin variables of the Feynman diagram. This innevitably means that the variable $A_{\alpha\beta}$ becomes part of an internal trace over spin variables. If we expand the corresponding response function $\chi(x) = \langle A(x)A(0)\rangle$ using Feynman diagrams, then we obtain

$$\chi(\tau) = \langle A(x)A(0)\rangle = \sum \text{closed linked two-vertex diagrams}$$



For example, in a non-interacting electron system, the imaginary time spin response function involves $A(x) = \mu_B\psi_\alpha{}^\dagger(x)\sigma_{\alpha\beta}\psi_\beta(x)$, so the corresponding response function is

$$\chi^{ab}(x-x') = \mu_B^2 \times$$



$$\begin{aligned}&= -\overbrace{\text{Tr}}^{\text{Trace over spin variables}}\left[\sigma^a\mathcal{G}(x-x')\sigma^b\mathcal{G}(x'-x)\right] \\ &= -\delta^{ab}2\mu_B^2\mathcal{G}(x-x')\mathcal{G}(x'-x)\end{aligned} \tag{10.16}$$

Now to analytically continue to real frequencies, we need to transform to Fourier space, writing

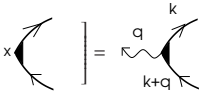
$$\chi(q) = \int d^4x e^{-iqx}\chi(x)$$

where the integral over time τ runs from 0 to β. This procedure converts the Feynman diagram from a real-space, to a momentum space Feynman diagram. At the measurement vertex at position x, the incoming and outgoing momenta of the fermion line give the following integral

$$\int d^4x e^{-iqx} e^{i(k_{in}-k_{out})x} = \beta V \delta^4(k_{out} - k_{in} + q).$$

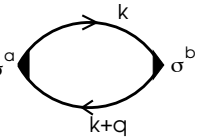
As in the case of the Free energy, the βV term cancels with the $1/(\beta V)\sum_k$ terms associated with each propogator, leaving behind one factor of $1/(\beta V) = T/V$ per internal momentum loop. Schematically, the effect of the Fourier transform on the measurement vertex at position x, is then

$$\int d^4x e^{-iqx}\left[\quad\right] = \tag{10.17}$$



For example, the momentum-dependent spin response function of the free electron gas is given by

$$\chi^{ab}(q) = \mu_B^2 \times$$



$$= -\frac{1}{\beta V}\sum_k \mathrm{Tr}\left[\sigma^a \mathcal{G}(k+q)\sigma^b \mathcal{G}(k)\right] = \delta^{ab}\chi(q) \tag{10.18}$$

where

$$\chi(\mathbf{q}, i\nu_r) = -2\mu_B^2 \int_{\mathbf{k}} T\sum_{i\omega_n} \mathcal{G}(\mathbf{k}+\mathbf{q}, i\omega_n + i\nu_r)\mathcal{G}(\mathbf{k}, i\omega_n) \tag{10.19}$$

When we carry out the Matsubara summation in the above expression by a contour integral, (see Chapter 9), we obtain

$$-T\sum_{i\omega_n} \mathcal{G}(\mathbf{k}+\mathbf{q}, i\omega_n + i\nu_r)\mathcal{G}(\mathbf{k}, i\omega_n) = -\int_{C'} \frac{dz}{2\pi i} f(z)\mathcal{G}(\mathbf{k}+\mathbf{q}, z+i\nu_r)\mathcal{G}(\mathbf{k}, z)$$
$$= \left(\frac{f_{\mathbf{k}} - f_{\mathbf{k}-\mathbf{q}}}{(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) - i\nu_r}\right), \tag{10.20}$$

where C' encloses the poles of the Green functions. Inserting this into (10.19), we obtain $\chi(\mathbf{q}, i\nu_r) = \chi(\mathbf{q}, z)|_{z=i\nu_r}$, *where*

$$\chi(\mathbf{q}, z) = 2\mu_B^2 \int_{\mathbf{k}} \left(\frac{f_{\mathbf{k}} - f_{\mathbf{k}-\mathbf{q}}}{(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) - i\nu_r}\right) \tag{10.21}$$

From this we can also read off the power-spectrum of spin fluctuations

$$\chi''(\mathbf{q}, \omega) = \mathrm{Im}\chi(\mathbf{q}, \omega + i\delta) = 2\mu_B^2 \int_{\mathbf{q}} \pi\delta(\epsilon_{\mathbf{q}+\mathbf{k}} - \epsilon_{\mathbf{k}} - \omega)\left[f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}\right] \tag{10.22}$$

When we come to consider conductivities, which involve the response function of current operators, we need to know how to deal with an operator that involves spatial, or temporal derivatives. To do this, it is convenient to examine the Fourier transform of the operator $A(x)$,

$$\int d^4x e^{-iqx}\psi^\dagger(x)A\psi(x) = \sum_k \psi^\dagger(k-q/2)A\psi(k+q/2)$$

In current operators, A is a function of gradient terms such as $\overleftrightarrow{\nabla}$ and $\overleftrightarrow{\partial}_t$. In this case, the use of the symmetrized gradient terms ensures that when we Fourier transform, the derivative terms are replaced by the midpoint momentum and frequency of the incoming or outgoing electron.

$$\int d^4x e^{-iqx}\psi^\dagger(x)A[-i\overleftrightarrow{\nabla}, i\overleftrightarrow{\partial}_t]\psi(x) = \sum_k \psi^\dagger(k-q/2)A(\mathbf{k}, i\omega_n)\psi(k+q/2)$$

for example, the current operator $\vec{J}(x) = \frac{e\hbar}{m}\left(-i\overleftrightarrow{\nabla}\right)$ becomes

$$J(q) = \sum_k e\vec{v}_{\mathbf{k}}\psi^\dagger(k-q/2)\psi(k+q/2),$$

where $\vec{v}_{\mathbf{k}} = \frac{\hbar\vec{k}}{m}$ is the electron velocity. For the thermal current operator $\vec{J}_t(\vec{x}) = \frac{\hbar^2}{m}\left(\overleftrightarrow{\nabla}\overleftrightarrow{\partial}_t\right)$,

$$\vec{J}_t(q) = \sum_k i\omega_n \frac{\hbar^2\vec{k}}{m}\psi^\dagger(k-q/2)\psi(k+q/2).$$

Example 10.1: Calculate the imaginary part of the dynamic susceptibility for non-interacting electrons and show that at low energies $\omega << \epsilon_F$,

$$\frac{\chi''(\mathbf{q}, \omega)}{\omega} = \begin{cases} \mu_B^2 \frac{N(0)}{v_F q} & (q \le 2k_F) \\ 0 & (q > 2k_F) \end{cases}$$

where $v_F = \hbar k_F/m$ is the Fermi velocity.

Solution: Starting with (10.22) In the low energy limit, we can write

$$\lim_{\omega\to 0}\frac{\chi''(\mathbf{q}, \omega)}{\omega} = 2\mu_B^2 \int_{\mathbf{q}} \delta(\epsilon_{\mathbf{q}+\mathbf{k}} - \epsilon_{\mathbf{k}})\frac{f_{\mathbf{k}+\mathbf{q}} - f_{\mathbf{k}}}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}}}$$
$$= 2\mu_B^2 \int_{\mathbf{q}} \delta(\epsilon_{\mathbf{q}+\mathbf{k}} - \epsilon_{\mathbf{k}})\left(-\frac{df}{d\epsilon_{\mathbf{k}}}\right) \tag{10.23}$$

Replacing

$$\int_{\mathbf{q}} \to \int d\epsilon N(\epsilon) \int_{-1}^{1} \frac{d\cos\theta}{2}$$

we obtain

$$\begin{aligned} \lim_{\omega\to 0} \frac{\chi''(\mathbf{q},\omega)}{\omega} &= 2\mu_B^2 N(0) \int_{-1}^{1} \frac{d\cos\theta}{2} \delta(\frac{q^2}{2m} + \frac{qk_F}{m}\cos\theta) \\ &= 2\mu_B^2 N(0) \frac{m}{2qk_F} = \mu_B^2 \left(\frac{N(0)}{v_F q}\right) \qquad (q < 2k_F) \end{aligned} \tag{10.24}$$

10.6 Spectroscopy: linking measurement and correlation

The spectroscopies of condensed matter provide the essential window on the underlying excitation spectrum, the collective modes and ultimately the ground-state correlations of the medium. Research in condensed matter depends critically on the creative new interpretations given to measurements. It is from these interpretations, that new models can be built, and new insights discovered, leading ultimately to quantitative theories of matter.

Understanding the link between experiment and the microscopic world is essential for theorist and experimentalist. At the start of a career, the student is often flung into a seminar room, where it is often difficult to absorb the content of the talk, because the true meaning of the spectroscopy or measurements is obscure to all but the expert - so it is important to get a rough idea of how and what each measurement technique probes - to know some of the pitfalls of interpretation - and to have an idea about how one begins to calculate the corresponding quantities from simple theoretical models.

Table. 10.1 Selected Spectroscopies .

	NAME	SPECTRUM	$\hat{A}$	Questions and Issues
ELECTRON	STM $\frac{dI}{dV}$	$\frac{dI}{dV}(\mathbf{x}) \propto A(\mathbf{x},\omega)\|_{\omega=e\mathbf{V}}$	$\psi(x)$	Surface probe. $T \sim 0$ measurement. Is the surface different?
	ARPES	$I(\mathbf{k},\omega) \propto f(-\omega)A(\mathbf{k},-\omega)$	$c_{\mathbf{k}\sigma}(t)$	$p_\perp$ unresolved. Surface probe. No magnetic field
	Inverse PES	$I(\omega) \propto \sum_{\mathbf{k}}[1-f(\omega)]A(\mathbf{k},\omega)$	$c^\dagger_{\mathbf{k}\sigma}(t)$	**p** unresolved. Surface probe.
SPIN	χ_{DC} Uniform Susceptibility	$\chi_{DC} = \int \frac{d\omega}{\pi\omega}\chi''(\mathbf{q}=0,\omega)$	M	$\chi \sim \frac{1}{T}$ local moments. $\chi \sim$ cons paramagnet
	Inelastic Neutron Scattering $\frac{d^2\sigma}{d\Omega d\omega}$	$S(\mathbf{q},\omega) = \frac{1}{1-e^{-\beta\omega}}\chi''(\mathbf{q},\omega)$	$S(\mathbf{q},t)$	What is the background? Quality of crystal?
	NMR Knight Shift $\frac{1}{T_1}$	$K_{contact} \propto \chi_{\rm local}$ $T\int_q F(\mathbf{q})\frac{\chi''(\mathbf{q},\omega)}{\omega}\Big\|_{\omega=\omega_N}$	$S(\mathbf{x},t)$	How is the orbital part subtracted? How does powdering affect sample?
CHARGE	Resistivity ρ	$\rho = \frac{1}{\sigma(0)}$	$\vec{j}(q=0)$	What is the resistance ratio? (R_{300}/R_0)
	Optical Conductivity	$\sigma(\omega) = \frac{1}{-i\omega}[\langle j(\omega')j(-\omega')\rangle]_0^\omega$	$\vec{j}(\omega)$	Reflectivity: How was the Kramer's Krönig done? Spectral weight transfer?

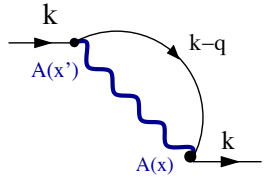
Fundamentally, each measurement is related to a given correlation function. This is seen most explicity in scattering experiments. Here, one is sending in one a beam of particles, and measuring the flux of outgoing particles at a given energy transfer E and momentum transfer $\mathbf{q}$. The ratio of outgoing to incoming particle flux determines the differential scattering cross-section

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{\text{Outward particle flux}}{\text{Inward particle flux}}$$

When the particles scatter, they couple to some microscopic variable $A(x)$ within the matter, such as the spin density in neutron scattering, or the particle field itself $A(x) = \psi(x)$ in photo-emission. The differential scattering cross-section this gives rise to what is, in essence a measure of the autocorrelation function of $A(x)$ at the wavevector $\mathbf{q}$ and frequency $\omega = E/\hbar$ inside the material,

$$\frac{d^2\sigma}{d\Omega d\omega} \sim \int d^4x \langle A(\mathbf{x},t)A(0)\rangle e^{-i(\mathbf{q}\cdot\mathbf{x}-\omega t)} = S(\mathbf{q},\omega)$$

Remarkably scattering probes matter at two points in space! How can this be? To understand it, recall that the differential scattering rate is actually an (imaginary) part of the forward scattering amplitude of the incoming particle. The amplitude for the incoming particle to scatter in a forward direction, contains the Feynman process where it omits a fluctuation of the quantity A at position x', travelling for a brief period of time as a scattered particle, before reabsorbing the fluctuation at x. The amplitude for the intermediate process is nothing more than



$$\text{amplitude} = \overbrace{\langle A(x)A(x')\rangle}^{\text{amplitude for fluctuation}} \underbrace{e^{i[\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')-\omega(\mathbf{t}-\mathbf{t}')]}}_{\substack{\text{amplitude for particle to scatter at x',}\\ \text{and reabsorb fluctuation at } x\,.}} \qquad (10.25)$$

(In practice, since the whole process is translationally invariant, we can replace x by $x - x'$ and set $x' = 0$.)

The relationship between the correlation function and scattering rate is really a natural consequence of Fermi's Golden rule, according to which

$$\frac{d^2\sigma}{d\Omega d\omega} \sim \Gamma_{i\to f} = \frac{2\pi}{\hbar}\sum_f p_i |\langle f|V|i\rangle|^2 \delta(E_f - E_i)$$

where p_i is the probability of being in the initial state $|i\rangle$. Typically, an incoming particle (photon, electron, neutron) with momentum $\mathbf{k}$ scatters into an outgoing particle state (photon, electron, neutron) with momentum $\mathbf{k}' = \mathbf{k} - \mathbf{q}$, and the system undergoes a transition from a state $|\lambda\rangle$ to a final

state $|\lambda'\rangle$:

$$|i\rangle = |\lambda\rangle|\mathbf{k}\rangle, \qquad |f\rangle = |\lambda'\rangle|\mathbf{k}'\rangle$$

If the scattering Hamiltonian with $V \sim g\int_{\mathbf{x}}\rho(\mathbf{x})A(\mathbf{x})$, where $\rho(\mathbf{x})$ is the density of the particle beam, then the scattering matrix element is

$$\langle f|\hat{V}|i\rangle = g\int_{\mathbf{x}'}\langle\mathbf{k}'|\mathbf{x}'\rangle\langle\lambda'|A(\mathbf{x}')|\lambda\rangle\langle\mathbf{x}'|\mathbf{k}\rangle = \frac{g}{V_o}\int_{\mathbf{x}'} e^{i\mathbf{q}\cdot\mathbf{x}'}\langle\lambda'|A(\mathbf{x}')|\lambda\rangle \qquad (10.26)$$

so the scattering rate is

$$\Gamma_{i\to f} = \frac{g^2}{V_0^2}\int_{\mathbf{x},\,\mathbf{x}'} p_\lambda\langle\lambda|A(\mathbf{x})|\lambda'\rangle\langle\lambda'|A(\mathbf{x}')|\lambda\rangle e^{-i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')}2\pi\delta(E_{\lambda'} - E_\lambda - \omega) \qquad (10.27)$$

where $p_\lambda = e^{-\beta(E_\lambda - F)}$ is the Boltzmann probability. Now if we repeat the spectral decomposition of the correlation function made in (10.9)

$$\int dt e^{i\omega t}\langle A(\mathbf{x},t)A(\mathbf{x}',0)\rangle = 2\pi\sum_{\lambda,\lambda'} p_\lambda\langle\lambda|A(x)|\lambda'\rangle\langle\lambda'|A(\mathbf{x}')|\lambda\rangle\delta(E_{\lambda'} - E_\lambda - \omega),$$

we see that

$$\begin{aligned}\Gamma_{i\to f} &\sim \frac{g^2}{V_0^2}\int_{\mathbf{x},\mathbf{x}'} dt e^{i\omega t}\langle A(\mathbf{x},t)A(\mathbf{x}',0)\rangle e^{-i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')} \\ &= \frac{g^2}{V_0}\int d^3x dt e^{-i(\mathbf{q}\cdot\mathbf{x}-\omega t)}\langle A(\mathbf{x},t)A(0)\rangle\end{aligned}$$

where the last simplification results from translational invariance. Finally, if we divide the transition rate by the incoming flux of particles $\sim 1/V_0$, we obtain the differential scattering cross-section.

For example, in an inelastic neutron scattering (INS) experiment, the neutrons couple to the electron spin density $A = S(x)$ of the material, so that

$$\frac{d^2\sigma}{d\Omega d\omega}(\mathbf{q},\omega) \sim \int d^4x\langle S_-(\mathbf{x},t)S_+(0)\rangle e^{-i(\mathbf{q}\cdot\mathbf{x}-\omega t)} \propto \frac{1}{1-e^{-\beta\omega}}\chi''(\mathbf{q},\omega)$$

where $\chi(\mathbf{q},\omega)$ is the dynamic spin susceptibility which determines the magnetization $M(\mathbf{q},\omega) = \chi(\mathbf{q},\omega)B(\mathbf{q},\omega)$ by a modulated magnetic field of wavevector $\mathbf{q}$, frequency ω. By contrast, in an angle resolved photo-emission (ARPES) experiment, incoming X-rays eject electrons from the material, leaving behind "holes", so that $A = \psi$ is the electron annihilation operator and the intensity of emitted electrons measures the correlation function

$$I(\mathbf{k},\omega) \sim \int d^4x\langle\psi^\dagger(x)\psi(0)\rangle e^{-i(\mathbf{k}\cdot\mathbf{x}-\omega t)} = \overbrace{\frac{1}{1+e^{\beta\omega}}}^{f(-\omega)} A(\mathbf{k},-\omega)$$

where the Fermi function replaces the Bose function in the fluctuation dissipation theorem.

10.7 Electron Spectroscopy

10.7.1 Formal properties of the electron Green function

The spectral decomposition carried out for a bosonic variable A is simply generalized to a fermionic variable such as $c_{\mathbf{k}\sigma}$. The basic electron "correlation" functions are

$$\begin{aligned}\langle c_{\mathbf{k}\sigma}(t)c^\dagger{}_{\mathbf{k}\sigma}(0)\rangle &= \int \frac{d\omega}{2\pi} G_>(\mathbf{k},\omega)e^{-i\omega t}\\ \langle c^\dagger{}_{\mathbf{k}\sigma}(0)c_{\mathbf{k}\sigma}(t)\rangle &= \int \frac{d\omega}{2\pi} G_<(\mathbf{k},\omega)e^{-i\omega t}\end{aligned} \tag{10.28}$$

called the "greater" and "lesser" Green functions. A spectral decomposition of these relations reveals that

$$\boxed{\begin{aligned}G_>(\mathbf{k},\omega) &= \sum_{\lambda,\zeta} p_\lambda |\langle\zeta|c^\dagger{}_{\mathbf{k}\sigma}|\lambda\rangle|^2 2\pi\delta(E_\zeta - E_\lambda - \omega)\\ G_<(\mathbf{k},\omega) &= \sum_{\lambda,\zeta} p_\lambda |\langle\zeta|c_{\mathbf{k}\sigma}|\lambda\rangle|^2 2\pi\delta(E_\zeta - E_\lambda + \omega)\end{aligned}}$$

describe the positive energy distribution functions for particles ($G_>$) and the negative energ distribution function for holes ($G_<$) respectively. By relabelling $\zeta \leftrightarrow \lambda$ in (10.29) it is straightforward to show that

$$G_<(\mathbf{k},\omega) = e^{-\beta\omega}G_>(\mathbf{k},\omega)$$

We also need to introduce the retarded electron Green function, given by

$$G_R(\mathbf{k},t) = -i\langle\{c_{\mathbf{k}\sigma}(t), c^\dagger{}_{\mathbf{k}\sigma}(0)\}\rangle\theta(t) = \int \frac{d\omega}{2\pi} G_R(\mathbf{k},\omega)e^{-i\omega t}$$

(note the appearance of an anticommutator for fermions and the minus sign pre-factor) which is the real-time analog of the imaginary time Green function

$$\mathcal{G}(\mathbf{k},\tau) = -\langle T\, c_{\mathbf{k}\sigma}(\tau)c^\dagger{}_{\mathbf{k}\sigma}(0)\rangle = T\sum_n \mathcal{G}(\mathbf{k},i\omega_n)e^{-i\omega_n\tau}$$

A spectral decomposition of these two functions reveals that they share the same power-spectrum and Kramer's Krönig relation, and can both be related to the generalized Green function

$$\mathcal{G}(\mathbf{k},z) = \int \frac{d\omega}{\pi}\frac{1}{z-\omega}A(\mathbf{k},\omega) \tag{10.29}$$

where

$$G_R(\mathbf{k},\omega) = \mathcal{G}(\mathbf{k},\omega+i\delta) = \int \frac{d\omega'}{\pi}\frac{1}{\omega-\omega'+i\delta}A(\mathbf{k},\omega)$$

$$\mathcal{G}(\mathbf{k},i\omega_n) = \mathcal{G}(\mathbf{k},z)|_{z=i\omega_n} = \int \frac{d\omega}{\pi}\frac{1}{i\omega_n-\omega}A(\mathbf{k},\omega'), \tag{10.30}$$

and the spectral function

$$\boxed{\begin{aligned}A(\mathbf{k},\omega) &= (1+e^{-\beta\omega})\sum_{\lambda,\zeta} p_\lambda |\langle\zeta|c^\dagger{}_{\mathbf{k}\sigma}|\lambda\rangle|^2\pi\delta(E_\zeta - E_\lambda - \omega)\\ &= \frac{1}{2}\left[G_>(\mathbf{k},\omega) + G_<(\mathbf{k},\omega)\right]\end{aligned}} \tag{10.31}$$

is the sum of the particle and hole energy distribution functions. From the second of (10.31) and (10.28), it follows that $A(\mathbf{k},\omega)$ is the Fourier transform of the anticommutator

$$\langle\{c_{\mathbf{k}\sigma}(t),\ c^\dagger{}_{\mathbf{k}\sigma}(0)\}\rangle = \int \frac{d\omega}{\pi}A(\mathbf{k},\omega)e^{-i\omega t} \tag{10.32}$$

At equal times, the commutator is equal to unity, $\{c_{\mathbf{k}\sigma},\ c^\dagger{}_{\mathbf{k}\sigma}\} = 1$, from which we deduce the normalization

$$\int \frac{d\omega}{\pi}A(\mathbf{k},\omega) = 1.$$

For non-interacting fermions, the spectral function is a pure delta-function, but in Fermi liquids the delta-function is renormalized by a factor Z and the remainder of the spectral weight is transfered to an incoherent background.

$$\frac{A(\mathbf{k},\omega)}{\pi} = Z_{\mathbf{k}}\delta(\omega - E_{\mathbf{k}}) + \text{background}$$

The relations

$$\begin{aligned}G_>(\mathbf{k},\omega) &= \frac{2}{1+e^{-\beta\omega}}A(\mathbf{k},\omega) = 2(1-f(\omega))A(\mathbf{k},\omega) \qquad \text{(particles)}\\ G_<(\mathbf{k},\omega) &= \frac{2}{1+e^{\beta\omega}}A(\mathbf{k},\omega) = 2f(\omega)A(\mathbf{k},\omega) \qquad \text{(holes)}\end{aligned} \tag{10.33}$$

are the fermion analog of the fluctuation dissipation theorem.

10.7.2 Tunneling spectroscopy

Tunneling spectroscopy is one of the most direct ways of probing the electron spectral function. The basic idea behind tunneling spectroscopy, is that a tunneling probe is close enough to the surface that electrons can tunnel through the forbidden region between the probe and surface material. Traditionally, tunneling was carried out using point contact spectroscopy, whereby a sharp probe is brought into contact with the surface, and tunneling takes place through the oxide layer separating probe and surface. With the invention of the Scanning Tunneling Microscope, by Gerd Binnig

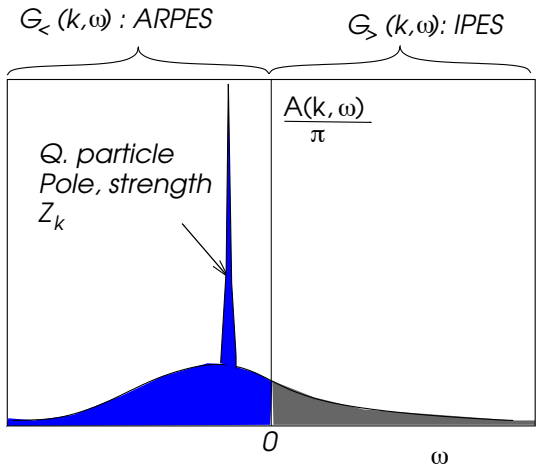


Figure 10.2: Showing the redistribution of the quasiparticle weight into an incoherent background in a Fermi liquid.

and Heinrich Rohrer in the 80's has revolutionized the field. In recent times, Seamus Davis has developed this tool into a method that permits the spectral function of electrons to be mapped out with Angstrom level precision across the surface of a conductor.

In the WKB approximation, the amplitude for an electron to tunnel between probe and surface is

$$t(x_1, x_2) \sim \exp\left[-\frac{1}{\hbar}\int_{x_1}^{x_2} \sqrt{2m[U(x)-E]}ds\right] \tag{10.34}$$

where the integral is evaluated along the saddle-point path between probe and surface. The exponential dependence of this quantity on distance means that tunneling is dominated by the extremal path from a single atom at the end of a scanning probe, giving rise to Angström - level spatial resolution.

The Hamiltonian governing the interaction between the probe and the sample can be written

$$\hat{V} = \sum_{\mathbf{k},\mathbf{k}'} t_{\mathbf{k},\mathbf{k}'}\left[c^\dagger_{\mathbf{k}\sigma} p_{\mathbf{k}'\sigma} + \text{H.c.}\right].$$

where $t_{\mathbf{k},\mathbf{k}'}$ is the tunnelling matrix element between the probe and substrate, $c^\dagger_{\mathbf{k}\sigma}$ and $p^\dagger_{\mathbf{k}\sigma}$ create electrons in the sample and the probe respectively. The tunneling current of electrons from probe to

sample is given by

$$i_{P\to S} = 2\pi \sum_{\mathbf{k},\mathbf{k}',\zeta,\zeta',\lambda,\lambda',\sigma} p_\lambda p_{\lambda'} |t_{\mathbf{k},\mathbf{k}'}|^2 |\langle\zeta,\zeta'|c^\dagger_{\mathbf{k}\sigma} p_{\mathbf{k}'\sigma}|\lambda,\lambda'\rangle|^2 \delta(E_\zeta + E_{\zeta'} - E_\lambda - E_{\lambda'})$$

where $|\lambda,\lambda'\rangle \equiv |\lambda\rangle|\lambda'\rangle$ and $|\zeta,\zeta'\rangle \equiv |\zeta\rangle|\zeta'\rangle$ refer to the joint many body states of the sample (unprimed) and probe (primed), and we have dropped $\hbar$ from the equation. This term creates electrons in the sample, leaving behind holes in the probe.

Now if we rewrite this expression in terms of the spectral functions of the probe and sample, after a little work, we obtain

$$i_{P\to S} = 4\pi \sum_{\mathbf{k},\mathbf{k}'} |t_{\mathbf{k},\mathbf{k}'}|^2 \int d\omega \frac{A_S(\mathbf{k},\omega)}{\pi}\frac{\tilde{A}_P(\mathbf{k},\omega)}{\pi}(1-f(\omega))f_P(\omega),$$

where $\tilde{A}_P(\mathbf{k},\omega)$ and $f_P(\omega)$ are the spectral function and distribution function of the voltage-biased probe. We have doubled the expression to account for spin. You can check the validity of these expressions by expanding the spectral functions using (10.31), but the expression is simply recognized as a product of matrix element, density of states and Fermi-Dirac electron and hole occupancy factors.

Similarly, the tunneling current of electrons from sample to probe is

$$\begin{aligned} i_{S\to P} &= 2\pi \sum_{\mathbf{k},\mathbf{k}',\zeta,\zeta',\lambda,\lambda',\sigma} p_\lambda p_{\lambda'} |t_{\mathbf{k},\mathbf{k}'}|^2 |\langle\zeta,\zeta'|p^\dagger_{\mathbf{k}'\sigma} c_{\mathbf{k}\sigma}|\lambda,\lambda'\rangle|^2 \delta(E_\zeta + E_{\zeta'} - E_\lambda - E_{\lambda'}) \\ &= 4\pi \sum_{\mathbf{k},\mathbf{k}'} |t_{\mathbf{k},\mathbf{k}'}|^2 \int d\omega \frac{A_S(\mathbf{k},\omega)}{\pi}\frac{\tilde{A}_P(\mathbf{k},\omega)}{\pi}[1-f_P(\omega)]f(\omega). \end{aligned} \tag{10.35}$$

Subtracting these two expressions, the total charge current $I = -|e|(i_{P\to S} - i_{S\to P})$ from probe to sample is

$$I = 4\pi|e| \sum_{\mathbf{k},\mathbf{k}'} |t_{\mathbf{k},\mathbf{k}'}|^2 \int d\omega \frac{A_S(\mathbf{k},\omega)}{\pi}\frac{\tilde{A}_P(\mathbf{k},\omega)}{\pi}[f(\omega) - f_P(\omega)]. \tag{10.36}$$

The effect of applying a voltage bias $V > 0$ to the probe is to lower the energy of the electrons in the probe, so that both the energy distribution function $f_P(\omega)$ and the spectral function of electrons in the probe $\tilde{A}_P(\mathbf{k},\omega)$ are shifted down in energy by an amount $|e|V$ with respect to their unbiased values, in other words $f_P(\omega) = f(\omega + |e|V)$ and $\tilde{A}_P(\mathbf{k},\omega) = A_P(\mathbf{k},\omega + |e|V)$, so that

$$I = 4\pi|e| \sum_{\mathbf{k},\mathbf{k}'} |t_{\mathbf{k},\mathbf{k}'}|^2 \int d\omega \frac{A_S(\mathbf{k},\omega)}{\pi}\frac{A_P(\mathbf{k},\omega + |e|V)}{\pi}[f(\omega) - f(\omega + |e|V)]. \tag{10.37}$$

We shall ignore the momentum dependence of the tunneling matrix elements, writing $|t|^2 = \overline{|t_{\mathbf{k},\mathbf{k}'}|^2}$, we obtain

$$I(V) = 2|e| \overbrace{2\pi|t|^2 N(0)}^{\Gamma} \int \frac{d\omega}{\pi}\frac{A_S(\omega)}{\pi}[f(\omega) - f(\omega + |e|V)]. \tag{10.38}$$

and

$$\begin{aligned} A_S(\omega) &= \sum_{\mathbf{k}} A_S(\mathbf{k},\omega) \\ N(\omega+|e|V) &= \sum_{\mathbf{k}} A_P(\mathbf{k},\omega+|e|V) \sim N(0) \end{aligned} \tag{10.39}$$

are the *local* spectral functions for the sample and probe, respectively. Typically, the probe is a metal with a featureless density of states, and this justifies the replacement $N(\omega) \sim N(0)$ in the above expression. The quantity $2\pi t^2 N(0) = \Gamma$ is the characteristic resonance broadening width created by the tunnelling out of the probe. If we now differentiate the current with respect to the applied voltage, we see that the differential conductivity

$$G(V) = \frac{dI}{dV} = \left(\frac{2e^2}{\hbar}\right)\Gamma \int \frac{d\omega}{\pi} A(S)(\omega) \overbrace{\left(-\frac{df(\omega+|e|V)}{d\omega}\right)}^{\sim\delta(\omega+|e|V)}$$

At low temperatures, the derivative of the Fermi function gives a delta function in energy, so that

$$G(V) = \left(\frac{4e^2\Gamma}{h}\right) A_S(\omega)|_{\omega=-|e|V}$$

Thus by mapping out the differential conductance as a function of position, it becomes possible to obtain a complete spatial map of the spectral function on the surface of the sample.

10.7.3 ARPES, AIPES and inverse PES

ARPES (angle resolved photoemission spectroscopy), AIPES (angle integrated photoemision spectroscopy) and inverse PES (inverse photo-electron spectrosopy) are the alternative ways of probing the hole and electron spectra in matter. The first two involve "photon in, electron out", the second "electron in, photon out". The coupling of radiation to light involves the dipole coupling term

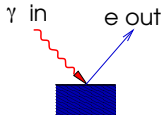
$$H_I = -\int d^3x \vec{j}(x)\cdot\vec{A}(x)$$

where $\vec{j}(x) = i\frac{e\hbar}{2m}\psi_\sigma{}^\dagger(x)\vec{\nabla}\psi_\sigma(x)$ is the paramagnetic electron current operator. Unlike STM or neutron scattering, this is a strongly coupled interaction, and the assumption that we can use the Golden Rule to relate the absorption to a correlation function is on much shakier ground. ARPES spectroscopy involves the absorption of a photon, and the emission of a photo-electron from the material. The interpretation of ARPES spectra is based on the "sudden approximation", whereby it is assumed that the dipole matrix element between the intial and final states has a slow dependence on the incoming photon energy and momentum, so that the matrix element is i.e

$$\langle\zeta,\mathbf{k}+\mathbf{q}|-\vec{j}\cdot\vec{A}|\lambda,\mathbf{q}\rangle \sim \Lambda(\mathbf{q},\hat{e}_\lambda)\langle\zeta|c_{\mathbf{k}\sigma}|\lambda\rangle$$

On the assumption that Λ is weakly energy and momentum dependent, we are able to directly relate the absorption intensity to the spectral density beneath the Fermi energy,

$$I_{ARPES}(\mathbf{k},\omega) \propto f(-\omega)A(\mathbf{k},-\omega)$$



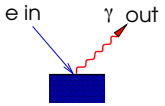
(10.40)

The appearance of the Fermi function masks states above the Fermi energy, and sometimes causes problems for the interpretation of ARPES spectra near the Fermi energy - particularly for the estimation of anisotropic, superconducting gaps. There is a large caveat to go with this equation: when photo-electrons escape from a surface, the component of their momentum perpendicular to the surface is modified by interactions with the surface. Consequently, ARPES spectroscopy can not resolve the momenta of the spectral function perpendicular to the surface. The other consideration about ARPES, is that it is essentially a surface probe - X-ray radiation has only the smallest ability to penetrate samples, so that the information obtained by these methods provides strictly a surface probe of the system.

In recent years, tremendous strides in the resolution of ARPES have taken place, in large part because of the interest in probing the electron spectrum of the quasi- two-dimensional cuprate superconductors. These methods have, for example, played an important role in exhibiting the anisotropic d-wave gap of these materials.

Inverse photo-electron spectroscopy probes the spectral function above the Fermi energy. At present, angle resolved IPES is not a as well developed, and most IPES work involves unresolved momenta, i.e

$$I_{IPES}(\omega) \propto \sum_{\mathbf{k}} [1-f(\omega)]A(\mathbf{k},\omega)$$



(10.41)

In certain materials, both PES and IPES spectra are available. A classic example is in the spectroscopy of mixed valent cerium compounds. In these materials, the Ce atoms have a singly occupied f-level, in the $4f^1$ configuration. PES spectroscopy is able to resolve the energy for the hole excitation

$$4f_1 \to 4f^0 + e^-, \qquad \Delta E_I = -E_f$$

where E_f is the energy of a single occupied $4f$ level. By contrast, inverse PES reveals the energy to add an electron to the $4f^1$ state,

$$e^- + 4f_1 \to 4f^2, \qquad \Delta E_{II} = E_f + U$$

where U is the size of the Coulomb interaction between two electrons in an f-state. By comparing these two absorption energies, it is possible to determine the size of the Coulomb interaction energy

10.8 Spin Spectroscopy

10.8.1 D.C. magnetic susceptibility

If one measures the static D. C. magnetization of a medium, one is measuring the magnetic response at zero wavevector $\mathbf{q} = 0$ and zero frequency $\omega = 0$. By the Kramer's Krönig relation encountered in (10.12), we know that

$$\chi_{DC} = \int \frac{d\omega}{\pi} \frac{\chi''(\mathbf{q}=0,\omega)}{\omega}$$

So the static magnetic susceptibility is an economy-class measurement of the magnetic fluctuation power spectrum at zero wavevector. Indeed, this link between the two measurements sometimes provides an important consistency check of neutron scattering experiments.

In static susceptibility measurements, there are two important limiting classes of behavior, Pauli paramagnetism, in which the susceptibility is derived from the polarization of a Fermi surface, and is weakly temperature dependent,

$$\chi \sim \frac{\mu_B^2}{\epsilon_F} \sim \text{constant.} \qquad \text{(Pauli paramagnetism)}$$

and Curie paramagnetism, produced by unpaired electrons localized inside atoms, commonly known as "local moments". where the magnetic susceptibilty is inversely proportional to the temperature, or more generally

$$\chi(T) \sim n_i \overbrace{\left(\frac{g^2\mu_B^2 j(j+1)}{3}\right)}^{M_{eff}^2} \times \frac{1}{T+T^*} \qquad \text{(local moment paramagnetism)}$$

where n_i is the concentration of local moments and M_{eff}^2 is the effective moment produced by a moment of total angular momentum j, with gyromagnetic ratio, g. T^* is a measure of the interaction between local moments. For Ferromagnets, $T^* = -T_c < 0$, and ferromagnetic magnetic order sets in at $T = T_c$, where the uniform magnetic susceptibility diverges. For antiferromagnetis, $T^* > 0$ gives a measure of the strength of interaction between the local moments.

10.8.2 Neutron scattering

Neutrons interact weakly with matter, so that unlike electrons or photons, they provide an ideal probe of the bulk properties of matter. Neutrons interact with atomic nucleii via an interaction of the form

$$\hat{H}_I = \alpha \int d^3x \psi^\dagger{}_N(x)\psi_N(x)\rho(x),$$

where $\rho(x)$ is the density of nucleii and $\psi_N(x)$ is the field of the neutrons. This interaction produces unpolarized scattering of the neutrons, with an inelastic scattering cross-section of the form (see example below),

$$\frac{d^2\tilde{\sigma}}{d\Omega dE} = \frac{k_f}{k_i}\left(\frac{\alpha m_N}{2\pi\hbar^2}\right)^2 \frac{S(\mathbf{q},E)}{2\pi}$$

where $S(\mathbf{q},E)$ is the autocorrelation function of nuclear density fluctuations in the medium. Where do these come from? They are of course produced by phonons in the crystal. The neutrons transfer energy to the nucleii by exciting phonons, and we expect that

$$S(\mathbf{q},E) \sim (1+n_B(E))\delta(E-\hbar\omega_{\mathbf{q}})$$

where $\omega_{\mathbf{q}\lambda}$ is the phonon dispersion spectrum inside the medium.

The second important interaction between neutrons and matter, is produced by the interaction between the nuclear moment and the magnetic fields inside the material. The magnetic moment of the neutron is given by

$$\vec{M} = \gamma\mu_N \frac{\vec{\sigma}}{2}$$

where $\gamma = -1.91$ is the gyromagnetic ratio of the neutron and $\mu_N = \frac{e\hbar}{2m_N}$ is the neutron Bohr magneton. The interaction with the fields inside the material is then given by

$$\hat{H}_I = \frac{\gamma\mu_N}{2}\int d^3x \psi^\dagger{}_N(x)\vec{\sigma}\psi_N(x)\cdot\vec{B}(x),$$

The magnetic field inside matter is produced by two sources- the dipole field generated by the electron spins, and the orbital field produced by the motion of electrons. We will only discuss the spin component here. The dipole magnetic field produced by spins is given by

$$B(\mathbf{x}) = \int d^3x' \underline{V}(\mathbf{x}-\mathbf{x}')\cdot\tilde{\mathbf{M}}(\mathbf{x}')$$

where $\vec{M}(\mathbf{x}) = \mu_{\mathbf{B}}\psi^\dagger(\mathbf{x})\tilde{\sigma}\psi(\mathbf{x})$ is the electron spin density and

$$\underline{V}(\mathbf{x}) = -\tilde{\nabla}\times\tilde{\nabla}\times\left(\frac{\mu_{\mathbf{0}}}{\mathbf{4}\pi|\mathbf{x}|}\right)$$

We can readily Fourier transform this expression, by making the replacements

$$\vec{\nabla} \to i\vec{q}, \qquad \frac{1}{(4\pi|x|)} \to \frac{1}{q^2} \tag{10.42}$$

so that in Fourier space,

$$\begin{aligned}\left[\underline{V}(\mathbf{q})\right]_{ab} &= \mu_0\left[\vec{q}\times\vec{q}\times\left(\frac{1}{q^2}\right)\right]_{ab} = \mu_0\left[\hat{q}\times\hat{q}\times\right]_{ab} \\ &= \mu_0\overbrace{\left[\delta_{ab}-\hat{q}_a\hat{q}_b\right]}^{\mathcal{P}_{ab}(\hat{q})}.\end{aligned} \tag{10.43}$$

The only effect of the complicated dipole interaction, is to remove the component of the spin parallel to the q-vector. The interaction between the neutron and electron spin density is simply written

$$H_I = g\int_{\mathbf{q}}\sigma_N(-\mathbf{q})\underline{\mathcal{P}}(\hat{\mathbf{q}})\cdot\vec{S}_e(\mathbf{q}), \qquad g = \mu_0\gamma\mu_N\mu_B$$

Apart from the projector term, this is essentially, a "point interaction" between the neutron and electron spin density. Using this result, we can easily generalize our earlier expression for the nuclear differential scattering to the case of unpolarized neutron scattering by replacing $\alpha \to g$, and identifying

$$S_\perp(\mathbf{q}, E) = \mathcal{P}_{ab}(\hat{q}) S^{ab}(\mathbf{q}, E)$$

as the projection of the spin-spin correlation function perpendicular to the q-vector. For unpolarized neutrons, the differential scattering cross-section is then

$$\frac{d^2\tilde{\sigma}}{d\Omega dE} = \frac{k_f}{k_i} r_o^2 S_\perp(\mathbf{q}, E)$$

where

$$\begin{aligned} r_0 &= \left(\frac{g m_N}{2\pi\hbar^2}\right) = \frac{\gamma}{2} \overbrace{\left(\frac{\mu_0}{4\pi}\right)}^{\frac{1}{4\pi\epsilon_0 c^2}} \frac{e^2}{m} \\ &= \left(\frac{\gamma}{2}\right) \frac{e^2_{cgs}}{mc^2} \end{aligned} \tag{10.44}$$

is, apart from the prefactor, the classical radius of the electron.

Example 10.2: Calculate, in the imaginary time formalism, the self-energy of a neutron interacting with matter and use this to compute the differential scattering cross-section. Assume the interaction between the neutron and matter is given by

$$\hat{H}_I = \alpha \int d^3x \psi^\dagger_N(x) \psi_N(x) \rho(x)$$

where $\psi_N(x)$ is the neutron field and $\rho(x)$ is the density of nuclear matter.

Solution:

We begin by noting that the the real-space self-energy of the neutron is given by

$$\Sigma(x - x') = \alpha^2 \langle \delta\rho(x) \delta\rho(x') \rangle \mathcal{G}(x - x')$$

where $\langle \delta\rho(x)\delta\rho(x')\rangle = \chi(x - x')$ is the real-time density response function of the nuclear matter. (Note that the minus sign in $-\alpha^2$ associated with the vertices is absent because the propagator used here $\langle \delta\rho(x)\delta\rho(0)\rangle$ contains no minus sign pre-factor.) If we Fourier transform this expression, we obtain

$$\begin{aligned} \Sigma(k) &= \frac{\alpha^2}{\beta V} \sum_q \mathcal{G}(k - q)\chi(q) \\ &= \alpha^2 \int_{\mathbf{q}} T \sum_{i\nu_n} \mathcal{G}(k - q)\chi(q) \end{aligned} \tag{10.45}$$

Carrying out the Matsubara summation, we obtain

$$\Sigma(\mathbf{k}, z) = \alpha^2 \int_{\mathbf{q}} \frac{dE'}{\pi} \frac{1 + n(E') - f_{\mathbf{k}-\mathbf{q}}}{z - (E_{\mathbf{k}-\mathbf{q}} + E')} \chi''(\mathbf{q}, E')$$

where $E_{\mathbf{k}}$ is the kinetic energy of the neutron and the Fermi function $f_{\mathbf{k}}$ of the neutron can be ultimately set to zero (there is no Fermi sea of neutrons), $f_{\mathbf{k}} \to 0$, so that

$$\Sigma(\mathbf{k}, z) = \alpha^2 \int_{\mathbf{q}} \frac{dE'}{\pi} \frac{1}{z - (E_{\mathbf{k}-\mathbf{q}} + E')} \overbrace{(1 + n(E'))\chi''(\mathbf{q}, E')}^{S(\mathbf{q},E)}$$

From the imaginary part of the self-energy, we deduce that the lifetime τ of the neutron is given by

$$\frac{1}{\tau} = \frac{2}{\hbar} Im\Sigma(\mathbf{k}, E_{\mathbf{k}} - i\delta) = \frac{2\alpha^2}{\hbar} \int_{\mathbf{k}'} S(\mathbf{k} - \mathbf{k}', E_{\mathbf{k}} - E_{\mathbf{k}'})$$

where we have changed the momentum integration variable from $\mathbf{q}$ to $\mathbf{k}' = \mathbf{k} - \mathbf{q}$. Splitting the momentum integration up into an integral over solid angle and an integral over energy, we have

$$\int_{\mathbf{k}'} = \int \left(\frac{m_N k_f}{8\pi^2\hbar^2}\right) dE' d\Omega'$$

from which we deduce that the mean-free path l of the neutron is given by

$$\frac{1}{l} = \frac{1}{v_N \tau} = \frac{1}{v_N} 2Im\Sigma(\mathbf{k}, E_{\mathbf{k}} - i\delta) = \int d\Omega_{\mathbf{k}'} dE_{\mathbf{k}'} \times \left[\frac{k_f}{k_i} \left(\frac{\alpha m_N}{2\pi\hbar^2}\right)^2 S(\mathbf{q}, E)\right]$$

where $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ and $E = E_{\mathbf{k}} - E_{\mathbf{k}'}$ and $v_N = \hbar k_i / m_N$ is the incoming neutron velocity.

Normally we write $l = 1/(n_i\sigma)$, where σ is the cross-section of each scatterer and n_i is the concentration of scattering centers. Suppose $\tilde{\sigma} = n_i\sigma$ is the scattering cross-section per unit volume, then $\tilde{\sigma} = 1/l$, so it follows that

$$\tilde{\sigma} = \frac{1}{v_N} 2Im\Sigma(\mathbf{k}, E_{\mathbf{k}} - i\delta) = \int d\Omega_{\mathbf{k}'} dE_{\mathbf{k}'} \times \left[\frac{k_f}{k_i} \left(\frac{\alpha m_N}{2\pi\hbar^2}\right)^2 S(\mathbf{q}, E)\right]$$

from which we may identify the differential scattering cross-section as

$$\frac{d^2\tilde{\sigma}}{d\Omega dE} = \frac{k_f}{k_i} \left(\frac{\alpha m_N}{2\pi\hbar^2}\right)^2 S(\mathbf{q}, E)$$

10.8.3 NMR

Knight Shift K

Nuclear Magnetic resonance, or "Magnetic resonance imaging" (MRI), as it is more commonly

referred to in medical usage, is the use of nuclear magnetic absorption lines to probe the local spin environment in a material. The basic idea, is that the Zeeman interaction of a nuclear spin in a magnetic field gives rise to a resonant absorption line in the microwave domain. The interaction of the nucleus with surrounding spins and orbital moments produces a "Knight shift" this line and it also broadens the line, giving it a width that is associated with the nuclear spin relaxation rate $1/T_1$.

The basic Hamiltonian describing a nuclear spin is

$$H = -\mu_n \vec{I}\cdot\vec{B} + H_{hf}$$

where $\vec{I}$ is the nuclear spin, μ_n is the nuclear magnetic moment. The term H_{hf} describes the "hyperfine" interaction between the nuclear spin and surrounding spin degrees of freedom. The hyperfine interaction between a nucleus at site i and the nearby spins can be written

$$\begin{aligned} H_{hf} &= -\vec{I}_i\cdot\vec{B}_{hf}(i) \\ \vec{B}_{hf}(i) &= \underline{A}_{\text{contact}}\cdot\vec{S}_i + \underline{A}_{\text{orbital}}\cdot\vec{L}_i + \sum_j \underline{A}_{\text{trans}}(i-j)\cdot S_j. \end{aligned} \tag{10.46}$$

where $B_{hf}(i)$ is an effective field induced by the hyperfine couplings. The three terms in this Hamiltonian are derived from a local contact interaction, with s-electrons at the same site, an orbital interaction, and lastly, a transfered hyperfine interaction with spins at neighboring sites. The various tensors $\underline{A}$ are not generally isotropic, but for pedagogical purposes, let us ignore the anisotropy.

The Knight shift - the shift in the magnetic resonance line, is basically the expectation value of the hyperfine field B_{hf} In a magnetic field, the electronic spins inside the material become polarized, with $\langle S_j\rangle \sim \chi B$, where χ is the magnetic susceptibility, so in the simplest situation, the Knight shift is simply a measure of the local magnetic susceptibility of the medium. n turn, a measure of the electron density of states $\langle N(\epsilon)\rangle$, thermally averaged around the Fermi energy, so

$$K \sim B_{hf} \sim \chi B \sim \langle N(\epsilon)\rangle B.$$

One of the classic indications of the development of a gap in the electron excitation spectrum of an electronic system, is the sudden reduction in the Knight shift. In more complex systems, where there are different spin sites, the dependence of the Knight shift can depart from the global spin susceptibility.

Another application of the Knight shift, is as a method to detect magnetic, or antiferromagnetic order. If the electrons inside a metal develop magnetic order, then this produces a large, field-independent Knight shift that can be directly related to the size of the ordered magnetic moment

$$K \sim \langle S_{\text{local}}\rangle$$

Unlike neutron scattering, NMR is able to distinguish between homogeneous and inhomogeneous magnetic order.

Relaxation rate $1/T_1$

The second aspect to NMR, is the broadening of the nuclear resonance. If we ignore all but the contact interaction, then the spin-flip decay rate of the local spin is determined by the Golden Rule,

$$\frac{1}{T_1} = \frac{2\pi}{\hbar} I^2 A^2_{contact} S_{+-}(\omega)\Big|_{\omega=\omega_N}$$

where ω_N is the nuclear resonance frequency and

$$\begin{aligned} S_{+-}(\omega) &= \int_{\mathbf{q}} [1+n_B(\omega)]\chi''_{+-}(\mathbf{q},\omega) \\ &\sim T\int \frac{d^3q}{(2\pi)^3}\frac{1}{\omega}\chi''_{+-}(\mathbf{q},\omega) \end{aligned} \tag{10.47}$$

at frequencies $\omega \sim \omega_N$, so for a contact interaction, the net nuclear relaxation rate is then

$$\frac{1}{T_1} = \frac{2\pi}{\hbar} I^2 A^2_{contact} \times T\int \frac{d^3q}{(2\pi)^3}\frac{1}{\omega}\chi''_{+-}(\mathbf{q},\omega)\Big|_{\omega=\omega_N}$$

In a classical metal, $\chi''(\omega)/\omega \sim N(0)^2$ is determined by the square of the density of states. This leads to an NMR relaxation rate

$$\frac{1}{T_1} \propto TN(0)^2 \sim \frac{k_B T}{\epsilon_F^2} \qquad \text{Korringa relaxation}$$

This linear dependence of the nuclear relaxation rate on temperature is name a "Korringa relaxation" law, after the Japanese theorist who first discovered it. Korringa relaxation occurs because the Pauli principle allows only a fraction fraction $TN(0) \sim T/\epsilon_F$ of the electrons to relax the nuclear moment. In a more general Fermi system, the NMR relaxation rate is determined by the thermally averaged square density of states.

$$\frac{1}{T_1} \sim T\int\left(-\frac{df(\omega)}{d\omega}\right)N(\omega)^2 \sim T\times[N(\omega\sim k_BT)]^2$$

In a wide class of anisotropic superconductors with lines of nodes along the Fermi surface, the density of states is a linear function of energy. One of the classic signatures of these line nodes across the Fermi surface is then a cubic dependence of $1/T_1$ on the temperature

$$\text{line nodes in gap } \Rightarrow N(\epsilon)\propto\epsilon, \qquad \Rightarrow \frac{1}{T_1}\propto T^3$$

In cases where the transferred hyperfine couplings are important, the non-locality introduces a momentum dependence into $A(\mathbf{k}) = \sum_{\vec{R}} A(\vec{R}_j)e^{-i\mathbf{k}\cdot\vec{R}_j}$these couplings. In this case,

$$\frac{1}{T_1} = \frac{2\pi}{\hbar} I^2 \times T\int \frac{d^3q}{(2\pi)^3}A(\mathbf{q})^2\frac{1}{\omega}\chi''_{+-}(\mathbf{q},\omega)\Big|_{\omega=\omega_N}$$

These momentum dependences can lead to radically different temperature dependences in the relaxation rate at different sites. One of the classic examples of this behavior occurs in the normal state of the high temperature superconductors. The active physics of these materials takes place in quasi-two dimensional layers of copper oxide, and the NMR relaxation rate can be measured at both the oxygen (O^{17}) and copper sites.

$$\left(\frac{1}{T_1}\right)_{Cu} \sim \text{constant}, \qquad \left(\frac{1}{T_1}\right)_{O} \sim \text{T},$$

The appearance of two qualitatively different relaxation rates is surprising, because the physics of the copper-oxide layers is thought to be described by a single-band model, with a single Fermi surface that can be seen in ARPES measurements. Why then are there two relaxation rates?

One explanation for this behavior has been advanced by Mila and Rice, who argue that there is indeed a single spin fluid, located at the copper sites. They noticed that whereas the copper relaxation involves spins at the same site, so that

$$A_{Cu}(\mathbf{q}) \sim \text{constant},$$

the spin relaxation rate on the oxygen sites involves a transfered hyperfine coupling between the oxygen p_x or p_y orbitals and the neigboring copper spins. The odd-parity of a p_x or p_y orbital means that the corresponding form factors have the form

$$A_{p_x}(\mathbf{q}) \sim \sin(q_x a/2).$$

Now high temperature superconductors are doped insulators. In the insulating state, cuprate superconductors are "Mott insulators", in which the spins on the Copper sites are antiferromagnetically ordered. In the doped metallic state, the spin fluctuations on the copper sites still contain strong antiferromagnetic correlations, and they are strongly peaked around $\vec{Q}_0 \sim (\pi/a, \pi/a)$, where a is the unit cell size. But this is precisely the point in momentum space where the transfered hyperfine couplings for the Oxygen sites vanish. The absence of the Korringa relaxation at the cupper sites is then taken as a sign that the copper relaxation rate is driven by strong antiferromagnetic spin fluctuations which do not couple to oxygen nucleii.

10.9 Electron Transport spectroscopy

10.9.1 Resistivity and the transport relaxation rate

One of the remarkable things about electron transport, is that one of the simplest possible measurements - the measurement of electrical resistivity, requires quite a sophisticated understanding of the interaction between matter and radiation for its microscopic understanding. We shall cover this relationship in more detail in the next chapter, however, at basic level, DC electrical resistivity can be interpreted in terms of the basic Drude formula

$$\sigma = \frac{ne^2}{m}\tau_{tr}$$

where $1/\tau_{tr}$ is the transport relaxation rate. In Drude theory, the electron scattering rate τ_{tr} is related to the electron mean-free path l via the relation

$$l = v_F \tau$$

where v_F is the Fermi velocity. We need to sharpen this understanding, for $1/\tau_{tr}$ is not the actual electron scattering rate, it is the rate at which currents decay in the material. For example, if we

consider impurity scattering of electrons with a scattering amplitude $u(\theta)$ which depends on the scattering angle θ, the electron scattering rate is

$$\frac{1}{\tau} = 2\pi n_i N(0)\overline{|u(\theta)|^2}$$

where

$$\overline{|u(\theta)|^2} = \int_{-1}^{1} \frac{d\cos\theta}{2}|u(\theta)|^2.$$

denotes the angular average of the scattering rate. However, as we shall see shortly, the transport scattering rate which governs the decay of electrical current contains an extra weighting factor:

$$\begin{aligned}\frac{1}{\tau_{tr}} &= 2\pi n_i N(0)\overline{|u(\theta)|^2(1-\cos\theta)} \\ \overline{|u(\theta)|^2(1-\cos\theta)} &= \int_{-1}^{1} \frac{d\cos\theta}{2}|u(\theta)|^2(1-\cos\theta). \end{aligned} \tag{10.48}$$

The angular weighting factor $(1-\cos\theta)$ derives from the fact that the change in the current carried by an electron upon scattering through an angle θe is $ev_F(1-\cos\theta)$. In other words, only large angle scattering causes current decay. For impurity scattering, this distinction is not very important but in systems where the scattering is concentrated near $q = 0$, such as scattering off ferromagnetic spin fluctuations, the $(1-\cos\theta)$ term substantially reduces the effectiveness of scattering as a source of resistance.

At zero temperature, the electron scattering is purely elastic, and the zero temperature resistance R_0 is then a measure of the elastic scattering rate off impurities. At finite temperatures, electrons also experience inelastic scattering, which can be strongly temperature dependent. One of the most important diagnostic quantities to characterize the quality of a metal is the resistance ratio - the ratio of resistance at room temperature to the resistance at absolute zero

$$RR = \text{Resistance Ratio} = \frac{R(300\text{K})}{R(0)}$$

The higher this ratio, the lower the amount of impurities and the higher the quality of sample. Hardware quality copper piping already has a resistance ratio of order a thousand! A high resistance ratio is vital for the observation of properties which depend on the coherent balistic motion of Bloch waves, such as de-Haas van Alphen oscillations or the development of anisotropic superconductivity, which is ultra-sensitive to impurity scattering.

With the small caveat of distinction between transport and scattering relaxation rates, the temperature dependent resistivity is an excellent diagnostic tool for understanding the inelastic scattering rates of electrons:

$$\rho(T) = \frac{m}{ne^2} \times \left(\frac{1}{\tau_{tr}(T)}\right)$$

There are three classic dependences that you should be familiar with:

- **Electron phonon scattering above the Debye temperature**

$$\frac{1}{\tau_{tr}} = 2\pi\lambda k_B T$$

Linear resistivity is produced by electron-phonon scattering at temperatures above the Debye temperature, where the coefficient λ is the electron-phonon coupling constant defined in the previous chapter. In practice, this type of scattering always tends to saturate once the electron mean-free path starts to become comparable with the electron wavelength. It is this type of scattering that is responsible for the weak linear temperature dependence of resistivity in many metals. A note of caution - for linear resistivity does not necessarily imply electron phonon scattering! The most well-known example of linear resitivity occurs in the normal state of the cuprate superconductors, but here the resistance does not saturate at high temperatures, and the scattering mechanism is almost certainly a consequence of electron-electron scattering.

- **Electron-electron or Baber scattering**

$$\frac{1}{\tau_{tr}} = \frac{\pi}{\hbar}\overline{|UN(0)|^2}N(0)(\pi k_B T)^2$$

where

$$\overline{|UN(0)|^2} = N(0)^2\int\frac{d\Omega_{\hat{\mathbf{k}}'}}{4\pi}|U(\mathbf{k}-\mathbf{k}')|^2(1-\cos(\theta_{\mathbf{k},\mathbf{k}'}))$$

is the weighted average of the electron-electron interaction $U(\mathbf{q})$. This quadratic temperature dependence of the inelastic scattering rate can be derived from the Golden rule scattering rate

$$\frac{1}{\tau_{tr}} = \frac{4\pi}{\hbar}\sum_{\mathbf{k}',\mathbf{k}''}|U(\mathbf{k}-\mathbf{k}')|^2(1-\cos\theta_{\mathbf{k},\mathbf{k}'})(1-f_{\mathbf{k}''})f_{\mathbf{k}'+\mathbf{k}''-\mathbf{k}}\delta(\epsilon_{\mathbf{k}'}+\epsilon_{\mathbf{k}''}-\epsilon_{\mathbf{k}'''})$$

where the $4\pi = 2\times 2\pi$ prefactor is derived from the sum over internal spin indices If we neglect the momentum dependence of the scattering amplitude, then this quantity is determined entirely by the three-particle phase space

$$\begin{aligned}\frac{1}{\tau_{tr}} &\propto \int d\epsilon' d\epsilon''(1-f(\epsilon'))(1-f(\epsilon''))f(-\epsilon'-\epsilon'')\\ &= T^2\int dxdy\left(\frac{1}{1-e^{-x}}\right)\left(\frac{1}{1-e^{-y}}\right)\left(\frac{1}{1-e^{-(x+y)}}\right) = \frac{\pi^2}{4}T^2 \qquad (10.49)\end{aligned}$$

In practice, this type of resistivity is only easily observed in strongly interacting electron materials, where it is generally seen to develop at low temperatures when a Landau Fermi liquid develops. The T^2 resistivity is a classic hallmark of Fermi liquid behavior.

- **Kondo spin-flip scattering**

In metals containing a dilute concentration of magnetic impurities, the spin-flip scattering generated by the impurities gives rise to a temperature dependent scattering rate of the form

$$\frac{1}{\tau_{tr}} \sim n_i\frac{1}{\ln^2\left(\frac{T}{T_K}\right)}$$

where T_K is the "Kondo temperature", which characterizes the characteristic spin fluctuation rate of magnetic impurity. This scattering is unusual, because it becomes stronger at lower temperatures, giving rise to a " resistance minimum" in the resistivity.

In heavy electron materials, the Kondo spin-flip scattering is seen at high temperatures, but once a coherent Fermi liquid is formed, the resistivity drops down again at low temperatures, ultimately following a T^2 behavior.

10.9.2 Optical conductivity

Probing the electrical properties of matter at finite frequencies requires the use of optical spectroscopy. In principle, optical spectroscopy provides a direct probe of the frequency dependent conductivity inside a conductor. The frequency dependent conductivity is defined by the relation

$$\vec{j}(\omega) = \sigma(\omega)\vec{E}(\omega)$$

Modern optical conductivity measurements can be made from frequencies in the infra -red of order $\omega \sim 10cm^{-1} \sim 1meV$ up to frequencies in the optical, of order $50,000cm^{-1} \sim 5eV$. The most direct way of obtaining the optical conductivity is from the reflectivity, which is given by

$$r(\omega) = \frac{1-n(\omega)}{1+n(\omega)} = \frac{1-\sqrt{\epsilon(\omega)}}{1+\sqrt{\epsilon(\omega)}},$$

where $n(\omega) = \sqrt{\epsilon(\omega)}$ is the diffractive index and $\epsilon(\omega)$ is the frequency dependent dielectric constant. Now $\epsilon(\omega) = 1+\chi(\omega)$ where $\chi(\omega)$ is the frequency dependent dielectric susceptibility. Now since the polarization $P(\omega) = \chi(\omega)E(\omega)$, and since the current is given by $j = \partial_t P$, it follows that $j(\omega) = -i\omega P(\omega) = -i\omega\chi(\omega)E(\omega)$, so that $\chi(\omega) = \sigma(\omega)/(-i\omega)$ and hence

$$\epsilon(\omega) = 1+\frac{\sigma(\omega)}{-i\omega}.$$

Thus in principle, knowledge of the complex reflectivity determines the opical conductivity.

In the simplest measurements, it is only possible to measure the intensity of reflected radiation, giving $|r(\omega)|^2$. More sophisticated " elipsometry" techniques which measure the reflectivity as a function of angle and polarization, are able to provide both the amplitude and phase of the reflectivity, but here we shall discuss the simplest case where only the amplitude $|r(\omega)|$ is available. In this situation, experimentalists use the "Kramers' Kronig" relationship which determines the imaginary part $\sigma_2(\omega)$ of the optical conductivity in terms of the real part, $\sigma_1(\omega)$, (Appendix A)

$$\sigma_2(\omega) = \omega\int_0^\infty\frac{d\omega'}{\pi}\frac{\sigma_1(\omega')}{\omega^2-\omega'^2}$$

This is a very general relationship that relies on the retarded nature of the optical response. In principle, this uniquely determines the dielectric function and reflectivity. However, since the range of measurement is limited below about $5eV$, an assumption has to be made about the high frequency behavior of the optical conductivity where normally, a Lorentzian form is assumed.

With these provisos, it becomes possible to invert the frequency dependent reflectivity in terms of the frequency dependent conductivity. We shall return in the next chapter for a consideration of the detailed relationship between the optical conductivity and the microscopic correlation functions. We will see shortly that the interaction of an electromagnetic field with matter involves the transverse vector potential, which couples to the currents in the material without changing the charge density. The optical conductivity can be related to the following response function

$$\sigma(\omega) = \frac{1}{-i\omega}\left[\frac{ne^2}{m} - \langle j(\omega)j(-\omega)\rangle\right]$$

This expression contains two parts - a leading diamagnetic part, which describes the high frequency, short-time response of the medium to the vector potential, and a second, "paramagnetic" part, which describes the slow recovery of the current towards zero. We have used the shorthand

$$\langle j(\omega)j(-\omega)\rangle = i\int_0^\infty dt d^3x \langle[\,j(x,t),\, j(0)]\rangle e^{i\omega t}$$

to denote the retarded response function for the "paramagnetic" part of the electron current density $j(x) = -i\frac{\hbar}{m}\psi^\dagger\vec{\nabla}\psi(x)$.

10.9.3 The f-sum rule.

One of the most valuable relations for the analysis of optical conductivity data, is the so-called "f-sum rule", according to which the total integrated weight under the conductivity spectrum is constrained to equal the plasma frequency of the medium,

$$\int_0^\infty \frac{d\omega}{\pi}\sigma(\omega) = \frac{ne^2}{m} = \omega_P^2\epsilon_0 \tag{10.50}$$

where n is the density of electronic charge and ω_P is the Plasma frequency. To understand this relation, suppose we apply a sudden pulse of electric field to a conductor

$$E(t) = E_0\delta(t), \tag{10.51}$$

then immediately after the pulse, the net drift velocity of the electrons is changed to $v = eE_0/m$, so the instantaneous charge current after the field pulse is

$$j(0^+) = nev = \frac{ne^2}{m}E_0, \tag{10.52}$$

where n is the density of carriers. After the current pulse, the electric current will decay. For example, in the Drude theory, there is a single current relaxation time rate τ_{tr}, so that

$$j(t) = \frac{ne^2}{m}e^{-t/\tau_{tr}}E_0 \tag{10.53}$$

and thus

$$\sigma(t-t') = \frac{ne^2}{m}e^{-(t-t')/\tau_{tr}}\theta(t-t') \tag{10.54}$$

and by Fourier transforming we deduce that

$$\sigma(\omega) = \int_0^\infty dt e^{i\omega t}\sigma(t) = \frac{ne^2}{m}\frac{1}{\tau_{tr}^{-1} - i\omega} \tag{10.55}$$

Actually, the f-sum rule does not depend on the detailed form of the curent relaxation. Using the instantaneous response in (10.52) we obtain

$$J(t=0^+) = E_o\sigma(t=0^+) = E_o\int_{-\infty}^\infty \frac{d\omega}{2\pi}e^{-i0^+}\sigma(\omega) = \frac{ne^2}{m}E_0 \tag{10.56}$$

is a consequence of Newton's law. It follows that (independently of how the current subsequently decays),

$$\int_0^\infty \frac{d\omega}{\pi}\sigma(\omega) = \frac{ne^2}{m} = \epsilon_0\omega_p^2 \tag{10.57}$$

where we have identified $\epsilon_0\omega_p^2 = \frac{ne^2}{m}$ with the plasma frequency ω_p of the gas. This relationship is called the f-sum rule, and it is important because it holds, independently of the details of how the current decays.

The important point about the f-sum rule, is that in principle, the total weight under the optical spectrum, is a constant, providing one integrates up to a high-enough energy. When the temperature changes however, it is possible for the spectral weight to redistribute. In a simple metal, the optical conductivity forms a simple "Drude peak" - Lorentzian of width $1/\tau_{tr}$ around zero frequency. In a semi-conductor, the weight inside this peak decays as $e^{-\Delta/T}$, where Δ is the semi-conducting gap. In a simple insulator, the balance of spectral weight must then reappear at energies above the direct gap energy Δ_g. By contrast, in a superconductor, the formation of a superconducting condensate causes the spectral weight in the optical conductivity to collapse into a delta-function peak.

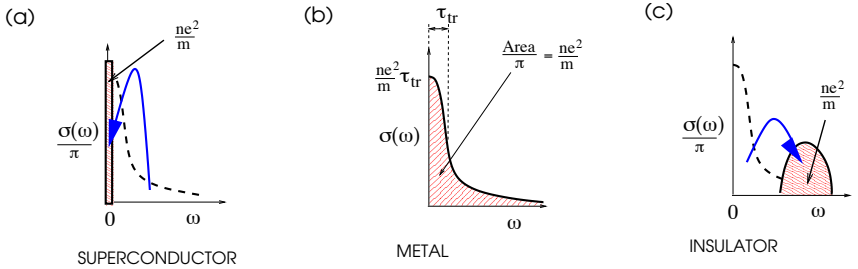


Figure 10.3: The f-sum rule. Illustrating (a) the spectral weight transfer down to the condensate in a superconductor (b) the Drude weight in a simple metal and (c) The spectral weight transfer up to the conduction band in an insulator.)

Appendix A: Kramer's Krönig relation

The Kramer's Krönig relation applies to any retarded linear response function, but we shall derive it here in special reference to the conductivity. In time, the current and electric field are related by the retarded response function

$$j(t) = \int_{-\infty}^{t} dt' \sigma(t-t')E(t') \tag{10.58}$$

which becomes $j(\omega) = \sigma(\omega)E(\omega)$ in Fourier space, where $\sigma(\omega)$ is the Fourier transform of the real-time response function $\sigma(t-t')$

$$\sigma(\omega) = \int_0^\infty dt e^{i\omega t}\sigma(t).$$

This function can be analytically extended into the upper-half complex plain ,

$$\sigma(z) = \sigma(x+iy) = \int_0^\infty dt e^{izt}\sigma(t) = . \int_0^\infty dt e^{ixt-yt}\sigma(t).$$

So long as z lies above the real axis, the real part $-yt$ of the exponent is negative, guaranteeing that the integral $\sigma(z)$ is both convergent and analytic. Provided $Imz_0 > 0$, then the conductivity can be written down using Cauchy's theorem

$$\sigma(z_0) = \int_{C'} \frac{dz}{2\pi i}\frac{\sigma(z)}{z-z_o}$$

where C' runs anti-clockwise around the point z_0. By distorting the contour onto the real axis, and neglecting the contour at infinity, it follows that

$$\sigma(z_0) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi i}\frac{\sigma(\omega')}{\omega'-z_0}$$

Taking $z_0 = \omega + i\delta$, and writing $\sigma(\omega+i\delta) = \sigma_1(\omega) + i\sigma_2(\omega)$ on the real axis, we arrive at the "Kramer's Krönig" relations

$$\begin{aligned}\sigma_2(\omega) &= -\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{\sigma_1(\omega')}{\omega'-\omega} = \omega\int_0^\infty \frac{d\omega'}{\pi}\frac{\sigma_1(\omega')}{\omega^2-\omega'^2}\\ \sigma_1(\omega) &= \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{\sigma_2(\omega')}{\omega'-\omega} = \int_0^\infty \frac{d\omega'}{\pi}\frac{\omega'\sigma_2(\omega')}{\omega^2-\omega'^2}\end{aligned} \tag{10.59}$$

10.10 Exercises

1. Spectral decomposition. The dynamic spin susceptibility of a magnetic system, is defined as

$$\chi(\mathbf{q}, t_1-t_2) = i\langle[S^-(\mathbf{q},t_1), S^+(-\mathbf{q},t_2)] > \theta(t_1-t_2) \tag{10.60}$$

where $S^\pm(\mathbf{q}) = S_x(\mathbf{q}) \pm iS_y(\mathbf{q})$ are the spin raising and lowering operators at wavevector $\mathbf{q}$, i.e

$$S^\pm(\mathbf{q}) = \int d^3 e^{-i\mathbf{q}\cdot\mathbf{x}} S^\pm(\mathbf{x}) \tag{10.61}$$

so that $S^-(\mathbf{q}) = [S^+(-\mathbf{q})]^\dagger$. The dynamic spin susceptibility determines the response of the magnetization at wavevector $\mathbf{q}$ in response to an applied magnetic field at this wavevector

$$M(\mathbf{q},t) = (g\mu_B)^2 \int dt' \chi(\mathbf{q}, t-t')B(t'). \tag{10.62}$$

(i)Make a spectral decomposition, and show that

$$\chi(\mathbf{q},t) = i\theta(t)\int \frac{d\omega}{\pi}\chi''(\mathbf{q},\omega)e^{i\omega t} \tag{10.63}$$

where $\chi''(\mathbf{q},\omega)$ (often called the "power-spectrum" of spin fluctuations) is given by

$$\chi''(\mathbf{q},\omega) = (1-e^{-\beta\omega})\sum_{\lambda,\zeta} e^{-\beta(E_\lambda - F)}|\langle\zeta|S^+(-\mathbf{q})|\lambda\rangle|^2\pi\delta[\omega-(E_\zeta - E_\lambda)] \tag{10.64}$$

and F is the Free energy.

(ii)Fourier transform the above result to obtain a simple integral transform which relates $\chi(\mathbf{q},\omega)$ and $\chi''(\mathbf{q},\omega)$. The correct result is a "Kramers Kronig" transformation.

(iii)In neutron scattering experiments, the inelastic scattering cross-section is directly proportional to a spectral function called $S(\mathbf{q},\omega)$,

$$\frac{d^2\sigma}{d\Omega d\omega} \propto S(\mathbf{q},\omega) \tag{10.65}$$

where $S(\mathbf{q},\omega)$ is the Fourier transform of a correlation function:

$$S(\mathbf{q},\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t}\langle S^-(\mathbf{q},t)S^+(-\mathbf{q},0)\rangle \tag{10.66}$$

By carrying out a spectral decomposition, show that

$$S(\mathbf{q},\omega) = (1+n(\omega))\chi''(\mathbf{q},\omega) \tag{10.67}$$

This relationship, plus the one you derived in part (i) can be used to completely measure the dynamical spin susceptibility via inelastic neutron scattering.

Bibliography

Chapter 11

Electron transport Theory

11.1 Introduction

Resistivity is one of the most basic properties of conductors. Surprisingly, Ohm's law

$$V = IR$$

requires quite a sophisticated understanding of the quantum many body physics for its understanding. In the classical electron gas, the electron current density

$$\vec{j}(x) = -ne\vec{v}(x)$$

is a simple c-number related to the average drift velocity $\vec{v}(x)$ of the negatively charged electron fluid. This is the basis of the Drude model of electricity, which Paul Drude introduced shortly after the discovery of the electron. Fortunately, many of the key concepts evolved in the Drude model extend to the a quantum description of electrons, where $\vec{j}(x)$ is an operator. To derive the current operator, we may appeal to the continuity equation, or alternatively, we can take the derivative of the Hamiltonian with respect to the vector potential,

$$\vec{j}(x) = -\frac{\delta H}{\delta \vec{A}(x)}$$

where

$$H = \int d^3x \left[\frac{1}{2m}\psi^\dagger(x)\left(-i\hbar\vec{\nabla} - e\vec{A}(x)\right)^2 \psi(x) - e\phi(x)\psi^\dagger(x)\psi(x)\right] + V_{INT}$$

where the Hamiltonian is written out for electrons of charge $q = e = -|e|$. Now only the Kinetic term depends on $\vec{A}$, so that

$$\vec{j}(x) = -\frac{ie\hbar}{2m}\psi^\dagger(x) \overleftrightarrow{\nabla} \psi(x) - \left(\frac{e^2}{m}\right)\vec{A}(x)\rho(x), \tag{11.1}$$

where $\overleftrightarrow{\nabla} = \frac{1}{2}\left(\vec{\nabla} - \overleftarrow{\nabla}\right)$ is the symmetrized derivative.

The discussion we shall follow dates back to pioneering work by Fritz London[1]. London noticed in connection with his research on superconductivity, that the current operator splits up into components, which he identified with the paramagnetic and diamagnetic response of the electron fluid:

$$\vec{j}(x) = \vec{j}_P(x) + \vec{j}_D(x) \tag{11.2}$$

where

$$\vec{j}_P(x) = -\frac{ie\hbar}{m}\psi^\dagger(x) \overleftrightarrow{\nabla} \psi(x) \tag{11.3}$$

and

$$\vec{j}_D(x) = -\left(\frac{e^2}{m}\right)\vec{A}(x)\rho(x). \tag{11.4}$$

Although the complete expression for the current density *is* invariant under gauge transformations $\psi(x) \to e^{i\phi(x)}\psi(x)$, $\vec{A}(x) \to \vec{A} - \frac{\hbar}{e}\vec{\nabla}\phi(x)$ the separate parts are not. However, in a *specific* gauge, such as the London or Coulomb gauge, where $\vec{\nabla}\cdot A = 0$, they do have physical meaning. We shall identify this last term as the term responsible for the diamagnetic response of a conductor, and the first term, the "paramagnetic current", is responsible for the decay of the current a metal.

In a non-interacting system, the current operator commutes with the Kinetic energy operator H_0 and is formally a constant of the motion. In a periodic crystal, electron momentum is replaced by the lattice momentum $\mathbf{k}$, which is, in the absence of lattice vibrations, a constant of the motion, with the result that the electron current still does not decay. What is the origin of electrical resistance?

There are then two basic sources of current decay inside a conductor:

- Disorder - which destroys the translational invariance of the crystal,
- Interactions - between the electrons and phonons, and between the electrons themselves, which cause the electron momenta and currents to decay.

The key response function which determines electron current is the conductivity, relating the Fourier component of current density at frequency ω, to the corresponding frequency dependent electric field,

$$\vec{j}(\omega) = \sigma(\omega)\vec{E}(\omega)$$

We should like to understand how to calculate this response function in terms of microscopic correlation functions.

The classical picture of electron conductivity was developed by Paul Drude, shortly after the discovery of the electron. Although his model was introduced before the advent of quantum mechanics, many of the basic concepts he introduced carry over to the quantum theory of conductivity. Drude introduced the the concept of the electron mean-free path l - the mean distance between scattering events. The characteristic timescale between scattering events is called the transport scattering time τ_{tr}. (We use the "tr" subscript to delineate this quantity from the quasiparticle scattering time τ, because not all scattering events decay the electric current.) In a Fermi gas, the characteristic velocity of electrons is the Fermi velocity and the mean-free path and transport scattering time are related by the simple relation

$$l = v_F\tau_{tr}$$

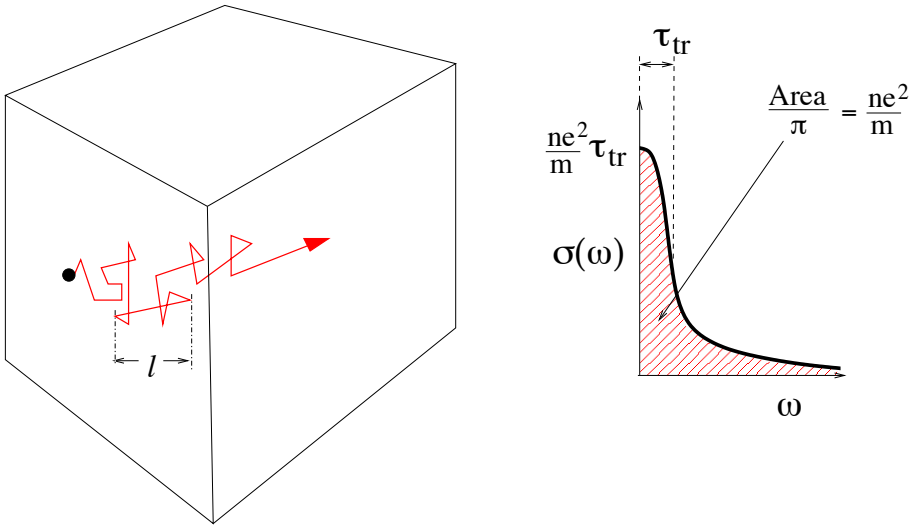


Figure 11.1: (a) Illustrating the diffusion of electrons on length-scales large compared with the mean-free path l, (b) The Drude frequency dependent conductivity. The short-time behavior of the current is determined by Newton's law, which constrains the area under the curve to equal $\int d\omega\sigma(\omega) = \pi\frac{ne^2}{m}$, a relation known as the f-sum rule.

The ratio of the mean-free path to the electron wavelength is the same order of magnitude as the ratio of the scattering time to the characteristic timescale associated with the Fermi energy $\hbar/\epsilon_F$ is determined by the product of the Fermi wavevector and the mean-free path

$$\frac{l}{\lambda_F} = \frac{k_F l}{2\pi} \sim \frac{\tau_{tr}}{\hbar/\epsilon_F} = \frac{\epsilon\tau_{tr}}{\hbar}$$

In very pure metals , the mean-free path of Bloch wave electrons l can be tens, even hundreds of microns, $l \sim 10^{-6}m$, so that this ratio can become as large as 10^4 or even 10^6. From this perspective, the rate at which current decays in a good metal is very slow on atomic time-scales.

There are two important aspects to the Drude model:

- the diffusive nature of density fluctuations,

- the Lorentzian line-shape of the optical conductivity

$$\sigma(\omega) = \frac{ne^2}{m}\frac{1}{\tau_{tr}^{-1} - i\omega}$$

Drude recognized that on length scales much larger than the mean-free path multiple scattering events induce diffusion into the electron motion. On large length scales, the current and density will be related by he diffusion equation,

$$\vec{j}(x) = -D\vec{\nabla}\rho(x),$$

where $D = \frac{1}{3}\frac{l^2}{\tau_{tr}} = \frac{1}{3}v_F^2\tau_{tr}$, which together with the continuity equation

$$\vec{\nabla}\cdot\vec{j} = -\frac{\partial\rho}{\partial t}$$

gives rise to the diffusion equation

$$\left[-\frac{\partial}{\partial t} + D\nabla^2\right]\rho = 0.$$

The response function $\chi(q,\nu)$ of the density to small changes in potential must be the Green's function for this equation, so that in Fourier space

$$[i\nu - Dq^2]\chi(q,\nu) = 1$$

from which we expect the response function and density-density correlation functions to contain a diffusive pole

$$\langle\delta\rho(q,\nu)\delta\rho(-q,-\nu)\rangle \sim \frac{1}{i\nu - Dq^2}$$

The second aspect of the Drude theory concerns the slow decay of current on the typical time-scale τ_{tr}, so that in response to an electric field pulse $E = E_0\delta(t)$, the current decays as

$$j(t) = e^{-\frac{t}{\tau_{tr}}}$$

In the last chapter, we discussed how, from a quantum perspective, this current is made up of two components, a diamagnetic component

$$j_{DIA} = -\frac{ne^2}{m}A = \frac{ne^2}{m}E_0, \qquad (t > 0)$$

and a paramagnetic part associated with the relax9ation of the electron wavefunction, which grows to cancel this component,

$$j_{PARA} = \frac{ne^2}{m}E_0(e^{-t/\tau_{tr}} - 1), \qquad (t > 0)$$

We should now like to see how each of these heuristic features emerges from a microscopic treatment of the conductivity and charge response functions. To do this, we need to relate the conductivity to a response fucntion - and this brings us to the Kubo formula.

11.2 The Kubo Formula

Lets now look again at the form of the current density operator. According to (11.1), it can divided into two parts

$$\vec{j}(x) = \vec{j}_P + \vec{j}_D \tag{11.5}$$

where

$$\begin{aligned} \vec{j}_P &= -\frac{i\hbar}{2m}\psi^\dagger(x)\overleftrightarrow{\nabla}\psi(x) \qquad \text{paramagnetic current} \\ \vec{j}_D &= -\frac{e^2}{m}\int d^3x\,\rho(x)\vec{A}(x) \qquad \text{diamagnetic current} \end{aligned} \tag{11.6}$$

are the "paramagnetic" and " diamagnetic" parts of the current. The total current operator is invariant under gauge transformations $\psi(x) \to e^{i\phi(x)}\psi(x)$, $\vec{A}(x) \to \vec{A} + \frac{\hbar}{e}\vec{\nabla}\phi(x)$ and speaking, the two terms in this expression for the current can't be separated in a gauge invariant fashion. However, in a specific gauge. We shall work in the London gauge

$$\vec{\nabla}\cdot\vec{A} = 0 \qquad \text{"London Gauge"}\,.$$

In this gauge, the vector potential is completely transverse, $\vec{q}\cdot\vec{A}(\vec{q}) = 0$. The equations of the electromagnetic field in the London Gauge are

$$\begin{aligned} \left(\frac{1}{c^2}\partial_t^2 - \nabla^2\right)\vec{A}(x) &= \mu_0\vec{j}(x) \\ -\nabla^2\phi(x) &= \frac{\rho(x)}{\epsilon_0} \end{aligned} \tag{11.7}$$

so that the potential field $\rho(x)$ is entirely determined by the distribution of charges inside the material, and the only independent external dynamic field coupling to the material is the vector potential. We shall then regard the vector potential as the only external field coupling to the material.

We shall now follow Fritz London's argument for the interpretation of these two terms. Let us carry out a thought experiment, in which we imagine a toroidal piece of metal, as in Fig. 11.2 in which a magnetic flux is turned on at $t = 0$, passing up through the conducting ring, creating a vector potential around the ring given by $A = A_0\theta(t) = \frac{\phi_0}{2\pi r}\theta(t)$, where r is the radius of the ring. The Electric field is related to the external vector potential via the relation

$$\vec{E} = -\frac{\partial\vec{A}}{\partial t} = -A_0\delta(t)$$

so $\vec{E} = -\vec{A}_o\delta(t)$ is a sudden inductively induced electrical pulse.

Suppose the system is described in the Schrödinger representation by the wavefunction $|\psi(t)\rangle$, then the current flowing after time t is given by

$$\langle\vec{j}(t)\rangle = \langle\psi(t)|\vec{j}_P|\psi(t)\rangle - \frac{ne^2}{m}A_o\theta(t) \tag{11.8}$$

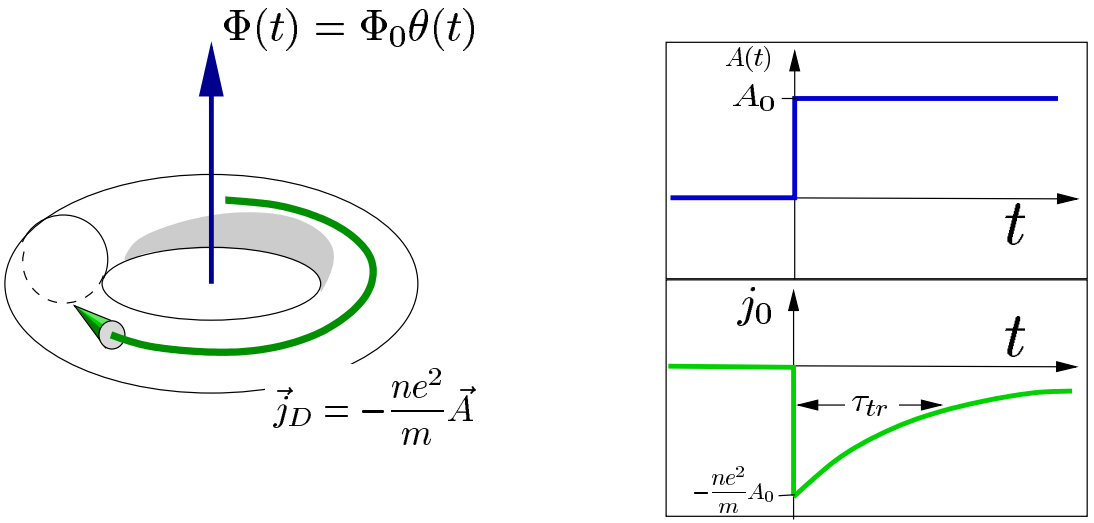


Figure 11.2: Schematic diagram to illustrate diamagnetic current pulse produced by a sudden change of flux through the conducting loop.

where we have assumed that $\langle\rho(x)\rangle = n$ is the equilibrium density of electrons in the material. We see that the second "diamagnetic" term switches on immediately after the pulse. This is nothing more than the diamagnetic response - the effect of the field induced by Faraday's effect. What is so interesting, is that this component of the current remains *indefinitely*, after the initial step in the flux through the toroid. But the current must decay! How?

The answer is that the initial "paramagnetic" contribution to the current starts to develop after the flux is turned on. Once the vector potential is present, the wavefunction $|\psi(t)\rangle$ starts to evolve, producing a paramagnetic current that rises and in a regular conductor, ultimately *exactly cancels* the time-independent diamagnetic current. From this point of view, the only difference between an insulator and a metal, is the timescale required for the paramagnetic current to cancel the diamagnetic component. In an insulator, this time-scale is of order the inverse (direct) gap Δ_g, $\tau \sim \hbar/\Delta_g$, whereas in a metal, it is the transport relaxation time $\tau \sim \tau_{tr}$.

These arguments were first advanced by Fritz London. He noticed that if, for some unknown reason the wavefunction of the material could become "rigid", so that it would not respond to the applied vector potential. In this special case, the paramagnetic current would never build up, and one would then have a perfect diamagnet - a superconductor. Lets now look at this in more detail.

We need to compute

$$\vec{j}(\vec{x},t) = \langle \vec{j}_P(x,t)\rangle - \frac{ne^2}{m}\vec{A}(x,t)$$

Now if we are to compute the response of the current to the applied field, we need to compute the build up of the paramagnetic part of the current. Here we can use linear response theory. The coupling of the vector potential to the paramagnetic current is simply $-\int d^3x \vec{j}(x)\cdot\vec{A}(x)$, so the response of this current is given by

$$\langle j_P^\alpha(t)\rangle = \int_{t'<t} d^3x'dt' i\langle[j_P^\alpha(x), j_P^\beta(x')]\rangle A^\beta(x') \tag{11.9}$$

In other words, we may write

$$\begin{aligned}\vec{j}(1) &= -\int d2\underline{Q}(1-2)\vec{A}(2)\\ Q^{\alpha\beta}(1-2) &= \frac{ne^2}{m}\delta^{\alpha\beta}\delta(1-2) - i\langle[j_P^\alpha(1), j_P^\beta(2)]\rangle\theta(t_1-t_2).\end{aligned} \tag{11.10}$$

The quantity $\underline{Q}(1-2)$ is the "London response" Kernel. In the most general case, this response is non-local in both space and time. In a metal, this response is non-local over a distance given by the electron mean-free path $l = v_F\tau_{tr}$. In a superconductor the response to the vector potential is non-local over the "Pippard coherence length", $\xi = v_F/\Delta$, where Δ is the superconducting gap. We can write the above result in Fourier space as

$$\vec{j}(q) = -\underline{Q}(q)\vec{A}(q)$$

where

$$Q^{\alpha\beta}(q) = \frac{ne^2}{m}\delta^{\alpha\beta} - i\langle[j^\alpha(q),\ j^\beta(-q)\rangle$$

and we have used the cavalier notation,

$$\langle[j^\alpha(q),\ j^\beta(-q)\rangle = \int d^3x\int_0^\infty dt\langle[j^\alpha(x,t),\ j^\beta(0)\rangle e^{-i(\vec{q}\cdot\vec{x}-\nu t)}.$$

Finally, if we write $\vec{E} = -\frac{\partial A}{\partial t}$, or $A(q) = \frac{1}{i\nu}E(q)$, we deduce that

$$\begin{aligned}\vec{j}(q) &= \underline{\sigma}(q)\vec{E}(q) \qquad\qquad \textbf{Kubo formula}\\ \sigma^{\alpha\beta}(q) &= -\frac{1}{i\nu}Q^{\alpha\beta}(q) = \frac{1}{-i\nu}\left\{\frac{ne^2}{m}\delta^{\alpha\beta} - i\langle[j^\alpha(q),\ j^\beta(-q)\rangle\right\}\end{aligned} \tag{11.11}$$

Now in practice, the high velocity of light means that $q = \nu/c << k_F$ is much shorter than an electronic wavevector, so that in electronic condensed matter physics, we may consider the limit $\vec{q} = 0$, writing $\sigma(\nu) = \sigma(\vec{q}=0,\nu)$. This is the quantity that is measured in optical conductivity measurements. The D.C. conductivity is given by the zero-frequency limit of the uniform conductivity, i.e. $\sigma_{DC} = Lt_{\nu\to 0}\sigma(\nu)$.

In a regular conductor, σ_{DC} is finite, which implies that $Q(\nu=0)=0$, so that in a conductor

$$i\langle[j^\alpha(q),\ j^\beta(-q)\rangle|_{q=0} = \frac{ne^2}{m}\delta^{\alpha\beta}$$

We shall see that this identity breaks down in a system with broken gauge invariance - and this is the origin of superconductivity. In a normal fluid however, we can use this identity to rewrite the expression for the conductivity as

$$\sigma^{\alpha\beta}(\nu) = \frac{1}{-i\nu}\left[-i\langle[j^\alpha(\nu'),\ j^\beta(-\nu')\rangle\right]_{\nu'=0}^{\nu'=\nu} \tag{11.12}$$

A practical calculation of conductivity depends on our ability to extract this quantity from the imaginary time response function. We can quickly generalize expression (11.10) to imaginary time, by replacing $i\langle[A(1),B(2)]\rangle \to \langle TA(1)B(2)\rangle$, so that in imaginary time,

$$\begin{aligned}\vec{j}(1) &= -\int d2\underline{Q}(1-2)\vec{A}(2), \qquad (1\equiv(\vec{x}_1,\tau_1))\\ Q^{\alpha\beta}(1-2) &= \frac{ne^2}{m}\delta^{\alpha\beta}\delta(1-2) - \langle Tj_P^\alpha(1)j_P^\beta(2)\rangle\end{aligned} \tag{11.13}$$

so that in Fourier space, our expression for the optical conductivity is given by

$$\sigma^{\alpha\beta}(i\nu_n) = -\frac{1}{\nu_n}\left[\ \langle Tj^\alpha(\nu')j^\beta(-\nu')\rangle\right]_{\nu'=0}^{\nu'=i\nu_n} \tag{11.14}$$

where we have used the short-hand notation

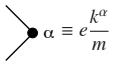
$$\langle Tj^\alpha(i\nu_n)j^\beta(-i\nu_n)\rangle = \int_0^\beta d\tau e^{i\nu_n\tau}\langle Tj^\alpha(\tau)j^\beta(0)\rangle$$

11.3 Drude conductivity: diagramatic derivation

In the last section we showed how the fluctuations of the electrical current can be related to the optical conductivity. Let us now see how these fluctuations can be computed using Feynman diagrams in a disordered electron gas with dispersion $\epsilon_{\mathbf{k}} = \frac{k^2}{2m}$. First, let us review the Feynman rules. We shall assume that we have taken the leading order effects of disorder into account in the electron propagator, denoted by

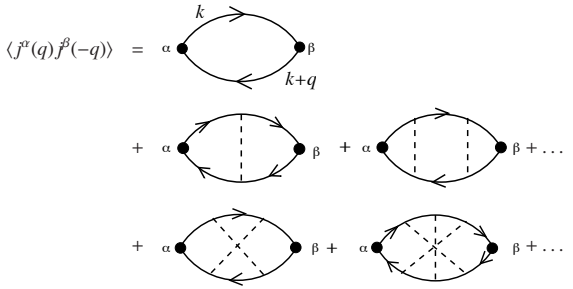
$$\longrightarrow = G(k) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}} + i\mathrm{sgn}\omega_n\frac{1}{2\tau}}$$

The current operator is $j^\alpha(q) = \sum e\frac{k^\alpha}{m}\psi^\dagger_{k-q/2\sigma}\psi_{k+q/2\sigma}$, which we denote by the vertex



$$\equiv e\frac{k^\alpha}{m}$$

The set of diagrams that represent the current fluctuations can then be written

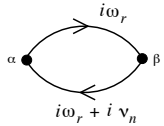


(11.15)

In the above expansion, we have identified three classes of diagrams. The first diagram, denotes the simplest contribution to the current fluctuation: we shall see shortly that this is already sufficient to capture the Drude conductivity. The second set of diagrams represent the leading impurity corrections to the current vertex: these terms take account of the fact that low-angle scattering does not affect the electric current, and it is these terms that are responsible for the replacement of the electron scattering rate τ by the transport relaxation rate τ_{tr}. We shall see that these terms vanish for isotropicaly scattering impurities, and justifying our neglect of these contributions in our warm-up calculation of the conductivity.

The last set of diagrams involve crossed impurity scattering lines - we have already encountered these types of diagrams in passing, and the momentum restrictions associated with crossed diagrams lead to a reduction factor of order $O(\frac{1}{k_F l}) \sim \frac{\lambda}{l}$, or the ratio of the electron wavelength to the mean-free path. These are the "quantum corrections" to the conductivity. These maximally crossed diagrams were first investigated by Langer and Neal in 1966, during the early years of research into electron transport , but it was not until the late 1970's that they became associated with the physics of electron localization - more on this later.

Using the Feynman rules, the first contribution to the current fluctuations is given by



$$\begin{aligned}\langle j^\alpha(i\nu_n)j^\beta(-i\nu_n)\rangle &= -2e^2T\sum_{\mathbf{k},i\omega_r}\frac{k^\alpha k^\beta}{m^2}G(\mathbf{k},i\omega_r+i\nu_n)G(\mathbf{k},i\omega_r)\end{aligned} \tag{11.16}$$

where the minus sign derives from the fermion loop and the factor of two derives from the sum over spin components. The difference between the fluctuations at finite and zero frequencies is then

$$\left[\langle j^\alpha(\nu)j^\beta(-\nu)\rangle\right]_0^{i\nu_n} = -2e^2T\sum_{\mathbf{k},i\omega_r}\frac{k^\alpha k^\beta}{m^2}\Big[\ G(\mathbf{k},i\omega_r+i\nu_n)G(\mathbf{k},i\omega_r)-\{i\nu_n\to 0\}\Big] \tag{11.17}$$

Now the amplitude at current fluctuations at any one frequency involves electron states far from the Fermi surface. However, the *difference* between the current fluctuations at two low frequencies cancels out most of these contributions, and the only important remaining contributions involve electrons with near the Fermi surface. This observation means that we can replace the momentum summation in (11.17) by an energy integral in which the density of states is approximated by a constant, and the limits are extended to infinity, as follows

$$\begin{aligned}\sum_{\mathbf{k}}\frac{k^\alpha k^\beta}{m^2}\Big[\ \dots\Big] &\to \int\frac{4\pi k^2dk}{(2\pi)^3}\int\frac{d\Omega_{\hat{\mathbf{k}}}}{4\pi}\frac{k^\alpha k^\beta}{m^2}\Big[\ \dots\Big]\\ &\to \delta^{\alpha\beta}\frac{v_F^2N(0)}{3}\int_{-\infty}^{\infty}d\epsilon\Big[\ \dots\Big]\end{aligned} \tag{11.18}$$

The London Kernel then becomes

$$\begin{aligned}Q^{\alpha\beta}(i\nu_n) &= 2\delta^{\alpha\beta}\frac{e^2v_F^2N(0)}{3}T\sum_{\omega_r}\times\\ &\quad 2\int_{-\infty}^{\infty}d\epsilon\left\{\overbrace{\left(\frac{1}{i\omega_r^+-\epsilon+i\mathrm{sgn}\omega_r^+/2\tau}\right)\left(\frac{1}{i\omega_r-\epsilon+i\mathrm{sgn}\omega_r/2\tau}\right)}^{\text{Poles on opposite side if }\omega_r^+>\omega_r}-\overbrace{\left(\quad i\nu_n\to 0\right)}^{\text{Poles on same side}}\right\}\end{aligned}$$

We can now carry out the energy integral by contour methods. We shall assume that $\nu_n > 0$. Now, provided that $i\omega_r^+ > 0$ and $i\omega_r < 0$, the first term inside this summation has poles on opposite sides of the real axis, at $\epsilon = i\omega_r + i/2\tau$ and $\epsilon = i\omega_r - 1/2\tau$, whereas the second term has poles on the same side of the real axis. Thus, when we complete the energy integral we only pick up contributions from the first term. (It doesn't matter which side of the real axis we complete the contour, but if we choose the contour to lie on the side where there are no poles in the second term, we are able to immediately see that this term gives no contribution.) The result of the integrals is then

$$\begin{aligned}Q^{\alpha\beta}(i\nu_n) &= \delta^{\alpha\beta}\overbrace{\frac{2e^2v_F^2N(0)}{3}}^{\frac{ne^2}{m}}T\sum_{0>\omega_r>-\nu_n,}\frac{2\pi i}{i\nu_n+i\tau^{-1}}\\ &= \delta^{\alpha\beta}\frac{ne^2}{m}\frac{\nu_n}{\tau^{-1}+\nu_n}\end{aligned} \tag{11.19}$$

Converting the London Kernel into the optical conductivity,

$$\sigma^{\alpha\beta}(i\nu_n) = \frac{1}{\nu_n}Q^{\alpha\beta}(i\nu_n) = \delta^{\alpha\beta}\frac{ne^2}{m}\frac{1}{\tau^{-1}-i(i\nu_n)}$$

Finally, analytically continuing onto the real axis, we obtain

$$\sigma^{\alpha\beta}(\nu + i\delta) = \frac{ne^2}{m}\frac{1}{\tau^{-1} - i\nu} \qquad \text{Transverse conductivity}$$

There are a number of important points to make about this result

- Our result ignores the effects of anisotropic scattering. To obtain these we need to include the "ladder" vertex corrections, which we will shortly see, replace

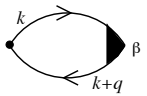
$$\frac{1}{\tau} \to \frac{1}{\tau_{tr}} = 2\pi n_i N(0)\overline{(1-\cos\theta)|u(\theta)|^2}, \tag{11.20}$$

  where the $(1-\cos\theta)$ term takes into account that small angle scattering does not relax the electrical current.

- Our result ignores localization effects that become important when $\frac{1}{k_F l} \sim 1$. In one or two dimensions, the effects of these scattering events accumulates at long distances, ultimately localizing electrons, no matter *how* weak the impurity scattering.

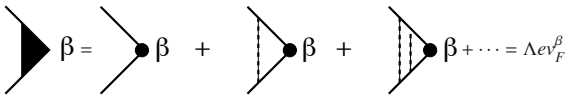
- Transverse current fluctuations are not diffusive - this is not surprising, since transverse current fluctuations do not involve any fluctuation in the charge density.

To improve our calculation, let us now examine the vertex corrections that we have so far neglected. Let us now re-introduce the "ladder" vertex corrections shown in (11.15). We shall write the current-current correlator as

$\langle j^\alpha(q) j^\beta(-q)\rangle =$ 

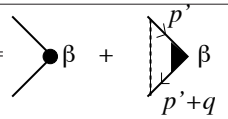
(11.21)

where the vertex correction is approximated by a sum of ladder diagrams, as follows



(11.22)

We shall re-write the vertex part as a self-consistent Dyson equation, as follows:

$e\Lambda v_F^\beta =$ 

(11.23)

where $q = (0, i\nu_n)$ and $p' = (\vec{p}\,', i\omega_r)$. The equation for the vertex part is then

$$ev_F^\beta \Lambda(\omega_r, \nu_n) = ev_F^\beta + n_i \sum_{\vec{p}\,'} |u(\vec{p} - \vec{p}\,')|^2 G(\vec{p}\,', i\omega_r^+) G(\vec{p}\,', i\omega_r)\Lambda(\omega_r, \nu_n) ev_F'^\beta. \tag{11.24}$$

Assuming that the vertex part only depends on frequencies, and has no momentum dependence, we may then write

$$\Lambda = 1 + \Lambda n_i \int \frac{d\cos\theta}{2}|u(\theta)|^2 \cos\theta \int \frac{d^3p'}{(2\pi)^3} G(\vec{p}\,', i\omega_r^+) G(\vec{p}\,', i\omega_r)$$

We can now carry out the integral over $\vec{p}\,'$ as an energy integral, writing

$$N(0)\int d\epsilon G(\epsilon, i\omega_r^+) G(\epsilon, i\omega_r) = N(0)\int d\epsilon \frac{1}{i\tilde{\omega}_n^+ - \epsilon}\frac{1}{i\tilde{\omega}_n - \epsilon}$$

where we use the short-hand

$$\tilde{\omega}_n = \omega_n + \text{sign}\omega_n(\frac{1}{2\tau}). \tag{11.25}$$

Carrying out this integral, we obtain

$$N(0)\int d\epsilon G(\epsilon, i\omega_r^+) G(\epsilon, i\omega_r) = \begin{cases} \pi N(0)\frac{1}{\nu_n + \tau^{-1}} & -\nu_n < \omega_r < 0 \\ 0 & \text{otherwise} \end{cases}$$

so that

$$\Lambda = 1 + \left(\frac{\bar{\tau}^{-1}}{\nu_n + \tau^{-1}}\right)\Lambda\theta_{\nu_n,\omega_r}$$

where $\bar{\tau}^{-1} = 2\pi n_i N(0)\overline{\cos\theta|u(\theta)|^2}$ and $\theta_{\nu_n,\omega_r} = 1$ if $-\nu_n < \omega_r < 0$ and zero otherwise, so that

$$\Lambda = \begin{cases} \frac{\nu_n + \tau^{-1}}{\nu_n + \tau_{tr}^{-1}} & -\nu_n < \omega_r < 0 \\ 1 & \text{otherwise} \end{cases} \tag{11.26}$$

where

$$\tau_{tr}^{-1} = \tau^{-1} - \bar{\tau}^{-1} = 2\pi n_i N(0)\overline{(1-\cos\theta)|u(\theta)|^2}.$$

when we now repeat the calculation, we obtain

$$\begin{aligned} Q^{\alpha\beta}(i\omega_n) &= \frac{ne^2}{m}\delta^{\alpha\beta} T\sum_{i\omega_r}\int_{-\infty}^{\infty} d\epsilon \left[G(\epsilon, i\omega_r^+)G(\epsilon, i\omega_r) - (i\nu_n \to 0)\right]\Lambda(i\omega_r, i\nu_n) \\ &= \frac{ne^2}{m}\delta^{\alpha\beta} T\sum_{i\omega_r}\frac{2\pi i}{i\nu_n + i\tau^{-1}}\frac{\nu_n + \tau^{-1}}{\nu_n + \tau_{tr}^{-1}} \end{aligned}$$

$$= \frac{ne^2}{m}\left(\frac{\nu_n}{\nu_n + \tau_{tr}^{-1}}\right)\delta^{\alpha\beta} \tag{11.27}$$

So making the analytic continuation to real frequencies, we obtain

$$\sigma(\nu + i\delta) = \frac{ne^2}{m}\frac{1}{\tau_{tr}^{-1} - i\nu}$$

Note that

- We see that transverse current fluctuations decay at a rate $\tau_{tr}^{-1} < \tau$. By renormalizing $\tau \to \tau_{tr}$, we take into account the fact that only backwards scattering relaxes the current. τ_{tr} and τ_{tr} are only identical in the special case of isotropic scattering. This distinction between scattering rates becomes particularly marked when the scattering is dominated by low angle scattering, which contributes to τ^{-1}, but does not contribute to the decay of current fluctuations.
- There is no diffusive pole in the transverse current fluctuations. This is not surprising, since transverse current fluctuations do not change the charge density.

11.4 Electron Diffusion

To display the presence of diffusion, we need to examine the density response function. Remember that a change in density is given by

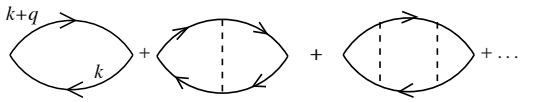
$$\langle \delta\rho(q)\rangle = i\langle[\rho(q),\rho(-q)]\rangle \overbrace{\delta\mu(q)}^{-eV(q)}$$

where V is the change in the electrical potential and

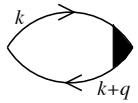
$$i\langle[\rho(q),\rho(-q)]\rangle = \int d^3x dt i\langle[\rho(x,t),\rho(0)]\rangle e^{-i\vec{q}\cdot\vec{x}+i\omega t}$$

We shall calculate this using the same set of ladder diagrams, but now using the charge vertex. Working with Matsubara frequencies, we have

$\langle\rho(q,i\nu_n)\rho(-q,-i\nu_n)\rangle$ =

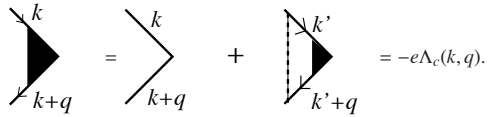


=



(11.28)

where the current vertex



$= -e\Lambda_c(k,q).$ (11.29)

Let us now rewrite (11.28) and (11.29) as equations. From (11.28) the density-density response function is given by

$$\langle\rho(q,i\nu_n)\rho(-q,-i\nu_n)\rangle = -2T\sum_k G(k+q)G(k)\Lambda_c(k,q).$$

From (11.29), the Dyson equation for the vertex is

$$\Lambda_c(k,q) = 1 + n_i\sum_{k'}|u(\mathbf{k}-\mathbf{k}')|^2 G(k'+q)G(k')\Lambda_c(k',q) \tag{11.30}$$

For convenience, we will assume point scattering, so that $u = u_0$ is momentum independent so that $\Lambda_c(k,q)$ only depends on k through its frequency component $i\omega_r$, so $\Lambda(k,q) = \Lambda(i\omega_r,q)$

$$\begin{aligned}\Lambda_c(i\omega_r,q) &= 1 + n_i u_0^2\sum_{k'} G(k'+q)G(k')\Lambda_c(i\omega_r,q)\\ &= 1 + \Pi(i\omega_r,q)\Lambda_c(i\omega_r,q)\end{aligned} \tag{11.31}$$

or

$$\Lambda_c(i\omega_r,q) = \frac{1}{1-\Pi(i\omega_r,q)}$$

where the polarization bubble is given by

$$\begin{aligned}\Pi(i\omega_r,q) &= n_i u_0^2\sum_{p'} G(k'+q)G(k')\\ &= n_i u_0^2 N(0)\int\frac{d\Omega}{4\pi}\int d\epsilon\frac{1}{i\tilde{\omega}_r^+ - (\epsilon+\vec{q}\cdot\vec{v}_F)}\frac{1}{i\tilde{\omega}_r - \epsilon}.\end{aligned} \tag{11.32}$$

(Note the use of the tilde frequencies, as defined in (11.25).) Now if $i\nu_n > 0$, then the energy integral in $\pi(i\omega_r,q)$ will only give a finite result if $-\nu_n < \omega_r < 0$. Outside this frequency range, $\pi(i\omega_r,q) = 0$ and $\Lambda_c = 1$. Inside this frequency range, $\Pi(i\omega_r,q) = \Pi(q)$ is frequency independent, and given by

$$\begin{aligned}\Pi(q) &= \overbrace{n_i u_0^2 N(0)}^{\tau^{-1}/(2\pi)}\int\frac{d\Omega}{4\pi}\frac{2\pi i}{i\nu_n + i\tau^{-1} + \vec{q}\cdot\vec{v}_F}\\ &= \int\frac{d\Omega}{4\pi}\frac{1}{1+\nu_n\tau - i\vec{q}\cdot\vec{v}_F\tau}\end{aligned} \tag{11.33}$$

Now we would like to examine the slow, very long wavelength charge flucations, which means we are interested in q small compared with the inverse mean-free path, $q << l^{-1} = 1/(v_F\tau)$, and in

frequencies that are much smaller than the inverse scattering length $\nu_n\tau << 1$. This permits us to expand Π in powers of $\vec{q}$. We shall take the first non-zero contribution, which comes in at order q^2. With these considerations in mind, we may expand Π as follows

$$\begin{aligned}\Pi(q) &= \int \frac{d\Omega}{4\pi}\left(1 - \nu_n\tau + i\vec{q}\cdot\vec{v}_F\tau + i^2(v_F\cdot\mathbf{q})^2\tau^2 + \ldots\right)\\ &= \left(1 - \nu_n\tau - \frac{v_F^2\tau}{3}q^2\tau + \ldots\right)\end{aligned} \tag{11.34}$$

where we neglect terms of order $O(q^2\nu_n)$. We may identify the combination $v_f^2\tau/3 = D$ in the second term with the diffusion constant D. Note that had we done this integral in d dimensions, the "3" in the denominator of the second term above would be replaced by d, but the general form for the diffusion constant in d dimensions is $D = v_f^2\tau/d$, so that in any dimension, we obtain

$$\Pi(q) = \left(1 - \nu_n\tau - Dq^2\tau + \ldots\right) \tag{11.35}$$

We then obtain

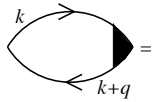
$$\Lambda_c(q) = \frac{1}{1-\Pi(q)} = \frac{\tau^{-1}}{\nu_n + Dq^2}, \qquad (-\nu_n < \omega_r < 0). \tag{11.36}$$

Summarizing then, the long-wavelength, low frequency charge vertex has the form

$$\Lambda_c(i\omega_r, q) = \begin{cases} \frac{i\tau^{-1}}{\nu_n + Dq^2}, & (-|\nu_n| < \mathrm{sgn}(\nu_n)\omega_r < 0)\\ 1 & \text{otherwise}\end{cases}$$

and thus the dynamic charge correlation function is given by

$$\langle\rho(q)\rho(-q)\rangle = \quad = -2N(0)T\sum_{i\omega_r}\int d\epsilon G(\epsilon, i\omega_r^+)G(\epsilon, i\omega_r)\Lambda_c(i\omega_r, q) \tag{11.37}$$



Now if we evaluate this quantity at zero frequency, $\nu_n = 0$, where $\Lambda_c = 1$, we obtain the static susceptibility

$$\begin{aligned}\chi_0 &= -2T\sum_{r,k}\frac{!}{(i\tilde{\omega}_r - \epsilon_k)^2}\\ &= 2\int d\epsilon N(\epsilon)\int\frac{d\omega}{2\pi i}f(\omega)\left\{\frac{1}{(\omega + i/(2\tau) - \epsilon)^2} - \frac{1}{(\omega - i/(2\tau) - \epsilon)^2}\right\}\\ &\qquad\qquad \overbrace{\qquad\qquad\qquad\qquad}^{-2iA(\epsilon,\omega)}\\ &= 2\int d\epsilon N(\epsilon)\int\frac{d\omega}{2\pi i}\frac{df(\omega)}{d\omega}\overbrace{\left\{\frac{1}{(\omega + i/(2\tau) - \epsilon)} - \frac{1}{(\omega - i/(2\tau) - \epsilon)}\right\}}\end{aligned}$$

$$= 2\int d\omega\left(-\frac{df(\omega)}{d\omega}\right)\overbrace{\int d\epsilon\frac{N(\epsilon)}{\pi}A(\epsilon,\omega)}^{=N(\omega)} = 2N(0) \qquad \text{unrenormalized} \tag{11.38}$$

so that the static charge susceptibility is unaffected by the disorder. This enables us to write

$$\langle\rho(q)\rho(-q)\rangle = \chi_0 - 2T\sum_{i\omega_r}\int N(\epsilon)d\epsilon\left[G(\epsilon, i\omega_r^+)G(\epsilon, i\omega_r)\Lambda_c(\omega_r, \nu_n) - \{\nu_n \to 0\}\right]$$

Since this intgeral is dominated by contributions near the Fermi energy, we can extend the energy integral over the whole real axis, replacing

$$\int N(\epsilon)d\epsilon \to N(0)\int_{-\infty}^{\infty}d\epsilon$$

enabling the energy integral to be carried out by contour methods, whereupon,

$$\begin{aligned}\langle\rho(q)\rho(-q)\rangle &= \chi_0 - 2TN(0)\sum_{i\omega_r}\int_{-\infty}^{\infty}d\epsilon\left[G(\epsilon, i\omega_r^+)G(\epsilon, i\omega_r)\Lambda_c(\omega_r, \nu_n) - \{\nu_n \to 0\}\right]\\ &= \chi_0 - \chi_0\overbrace{\left(\frac{\nu_n}{\nu_n + \tau^{-1}}\right)}^{\to\nu_n\tau}\left[\frac{\tau^{-1}}{\nu_n + Dq^2}\right]\end{aligned}$$

where, again, in the last step we have assumed $|\nu_n|\tau << 1$. The Matsubara form for the charge susceptibility is then

$$\chi_o(\vec{q}, i\nu_n) = \chi_0\frac{Dq^2}{|\nu_n| + Dq^2}$$

Analytically continuing this result, we finally obtain

$$\boxed{\chi(\vec{q}, \nu + i\delta) = \chi_0\left(\frac{Dq^2}{Dq^2 - i\nu}\right)} \tag{11.39}$$

. Note that:

- Density fluctuations are diffusive. Indeed, we could have anticipated the above form on heuristic grounds. The solution of the diffusion equation $D\nabla^2\rho = \frac{\partial\rho}{\partial t}$ is, in Fourier space,

  $$\rho(\vec{q}, \nu) = \frac{1}{Dq^2 - i\nu}\rho(q)$$

  where $\rho(q)$ is the Fourier transform of the initial charge distribution. If we require $\rho(\vec{q}, \nu = 0) = \chi_0 U(\vec{q})$, where $U(\vec{q})$ is the Fourier transform of the applied potential, then this implies (11.39)

- The order of limits is important, for whereas

$$\lim_{q\to 0}\lim_{\nu\to 0}\chi(q,\nu) = \chi_0$$

which is the response to a static potential of large, but finite wavelength,

$$\lim_{\nu\to 0}\lim_{q\to 0}\chi(q,\nu) = 0$$

which states that the response to a uniform potential of vanishingly small frequency is zero. The difference in these two response functions is due to the conservation of charge - if one wants to change the charge density in one place, it can only be done by redistributing the charge. If one applies a static uniform potential, the charge density does not change.

- We can use these results to deduce the longitudinal conductivity - the current response to a longitudinal electric field for which $\vec{q}\cdot\vec{E}\neq 0$. Let $\phi(q)$ be the electric potential, then $\delta\rho(q) = \chi(q)e\phi(q)$, so that

$$\begin{aligned}\delta\rho(q) = \chi_0\frac{Dq^2}{Dq^2-i\nu}e\phi(q) &= -\chi_0\frac{Di\vec{q}\cdot\overbrace{(i\vec{q}\phi(q))}^{\vec{\nabla}\phi=-\vec{E}(q)}}{Dq^2-i\nu}\\ &= \chi_0\left(\frac{Di\vec{q}}{Dq^2-i\nu}\right)\cdot\vec{E}(q)\end{aligned}\qquad(11.40)$$

Now since $\frac{\partial\rho}{\partial t}\equiv -i\nu\rho(q)$, it follows that

$$\dot{\rho}(q) = e\chi_0\left(\frac{Dv\vec{q}}{Dq^2-i\nu}\right)\cdot\vec{E}(q).\qquad(11.41)$$

Now by continuity, $e\frac{\partial\rho}{\partial t} = -\vec{\nabla}\cdot\vec{j}(q) = -i\vec{q}\cdot\vec{j}(q)$, where $\vec{j}$ is the charge current, so by comparing with (11.41) we deduce that the longitudinal current is

$$j_L(q) = e^2\chi_0 D\left(\frac{i\nu}{i\nu-Dq^2}\right)\vec{E}(q),$$

so the longitudinal conductivity contains a diffusive pole

$$\sigma_{LONG}(q) = e^2\chi_0 D\left(\frac{i\nu}{i\nu-Dq^2}\right).$$

Note also that at $q=0$, $\sigma = e^2\chi_0 D$, which can be written as the Einstein relation

$$\sigma = e^2\chi_0 D = \frac{ne^2}{m}\tau \qquad \text{Einstein Relation}$$

11.5 Weak Localization

We should like to finish our brief introduction to electron transport by touching on the concept of electron localization. The disorder that has been considered in this chapter is weak and the electron states we have considered are delocalized. We have remarked on a few occasions that disorder is like a kind of "attractive" but infinitely retarded interaction, and like other attractive interactions, it has the capacity to induce new kinds of collective behavior amongst the electrons. Infact, disorder actually gives rise to collective interference effects within the electron gas, which ultimately lead to the localization of the electron wavefunction. This idea was first proposed by Anderson in the late 1950's, but it took two decades for the idea to gain acceptance in the physics community. Our modern understanding of electron localization was greatly aided by a conceptual break-through on this problem made by Thouless who proposed that the resistance of a material, or rather, the inverse resistance, the conducance $G = 1/R$ is a function of scale. Thouless's idea, initially proposed for one dimension, was taken up by the so called "Gang of Four", Abrahams, Anderson Licciardello and Ramakrishnan and extended to higher dimensions leading to the modern "scaling theory" of localization. One of the ideas that emerged from this break-through, is that electron localization results from the coherent interference between electron waves, which at long-distances ultimately builds up to produce a disorder-drive metal-insulator transition - a kind of phase transition in which the order parameter is the conductance. Like all phase transitions, localization is sensitive to the dimensionality. Whereas in three dimensions, electron localization requires that the disorder exceed a critical value, in two and one dimension, an arbitrarily small amount of disorder is sufficient to localize electrons, and the leading order effects of localization can already be seen in weakly disordered materials. These ideas can all be developed for weakly disordered conductors by a simple extention of the Feynman diagram methods we have been using.

To develop a rudimentary conceptual understanding of electron localization, we shall follow a heuristic argument by Altshuler, Aronov, Larkin and Khmelnitskii[??], (see also Bergman [??]) who pointed out that weak localization results from the constructive interference between electrons passing along time-reversed paths. Consider the amplitude for an electron to return to its starting point. In general, it can do this by passing around a a sequence of scattering sites labelled 1 through n, as shown in Fig. 11.3, where we identify $n\equiv 1$ as the same scattering site. The amplitude for scattering around this loop is

$$A_P = G_R(n,n-1)G_R(n-1,n-2)\ldots G_R(2,1)$$

where

$$G_R(\vec{x}_1,\vec{x}_2) = \int\frac{d^dk}{(2\pi)^d}\frac{1}{\omega-\epsilon_{\mathbf{k}}+i\delta}e^{i\vec{k}\cdot(\vec{x}_1-\vec{x}_2)}$$

is the retarded propagator describing the amplitude for an electron of frequency ω to propagate between two sites. Now for each path P, there is a corresponding time-reversed path $\tilde{P}$. The amplitude for the same electron to follow $\tilde{P}$ starting at $1\equiv n$, is

$$A_{\tilde{P}} = G_R(1,2)G_R(2,3)\ldots G_R(n-1,n)$$

The total propability associated with passage along both paths is given by

$$P = |A_P + A_P|^2 = |A_P|^2 + |A_P|^2 + 2\mathrm{Re}[A_P^* A_P]$$

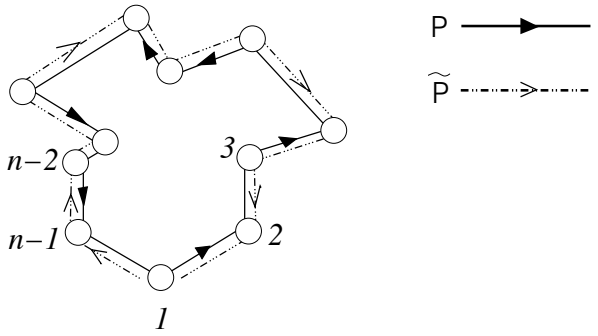


Figure 11.3: Scattering of an electron around two time-reversed paths

Now if $A_P = \sqrt{p_1}e^{i\phi_1}$ and $A_{\tilde{P}} = \sqrt{p_2}e^{i\phi_2}$ then total probability to scatter back to the starting point via the two paths,

$$p_{TOT} = p_1 + p_2 + 2\sqrt{p_1 p_2}\cos(\phi_2 - \phi_1).$$

contains an interference term $2\sqrt{p_1 p_2}\cos(\phi_2-\phi_1)$. If the two paths were unrelated, then the impurity average of interference term would be zero, and we would expect $\overline{P} = p_1 + p_2$. However! The two paths *are* related by time-reversal, so that $A_{\tilde{P}} = A_P$, with precisely the same magnitude and phase, and so the two processes always *constructively interfere*,

$$p_{TOT} = 4p_1$$

Without the interference term $p_{TOT} = 2p_1$, so we see that constructive interference between time-reversed paths doubles the return probabilty.

This means that an electron that enters into a random medium has an quantum-mechanically *enhanced* probability of returning to its starting point - quantum electrons "bounce back" twice as often as classical electrons in a a random medium! The same phenomenon causes the light from a car's headlamps to reflect backwards in a Fog. These effects tend to localize waves - causing light localization in the case of fog - and electron localization in disordered conductors. We shall see that the return probability is enhanced in lower dimensions, and in one, or two dimensions, these effects innevitably lead to the localization of electrons, for arbitrarily small amounts of disorder.

Let us now make a diagramatic identification of these interference terms. The complex conjugate of the retarded propagator is the advanced propagator

$$G_R(2-1,\omega)^* = G(2-1,\omega+i\delta)^* = G(2-1,\omega-i\delta) == G_A(2-1,\omega)$$

so the interference term

$$A^*_{\tilde{P}}A_P = \prod_{j=1}^{n-1} G_R(j+1,j;\omega)G_A(j+1,j;\omega)$$

which is represented by a "ladder diagram" for repeated scattering of electron pairs. The sum

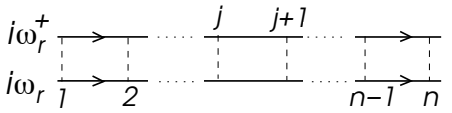


Figure 11.4: n-th order contribution to the "Cooperon"

of all such diagrams is called a "Cooperon", because of its similarity to the pair susceptibility in superconductivity. Notice that the lower electron line involves the advanced propagator G_A, whereas the upper involves the retarded propagator G_R. In the Matsubara approach the distinction between these two propagators is enforced by running a frequency $i\omega_r^+ \equiv i\omega_r + i\nu_n$ along the top line, and a frequency $i\omega_r$ along the bottom. When ν_n is analytically continued and ultimately set to zero, this enforces the distinction betwen the two propagators. Now if we twist the Cooperon around, we see that it is equivalent to a maximally crossed, or "Langer-Neal" diagram

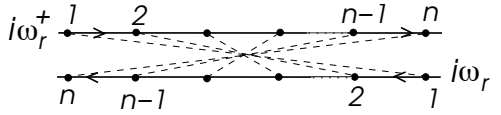
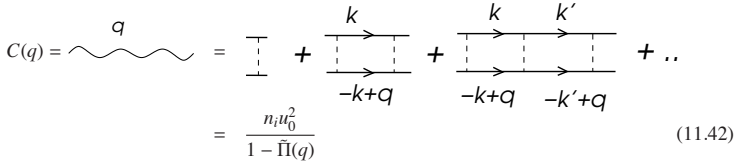


Figure 11.5: A twisted cooper diagram forms a maximally crossed diagram.

Let us now compute the amplitudes associated with these localization corrections to the conductivity. We begin by denoting the Cooperon by a sum of ladder diagrams



(11.42)

where

$$\bar{\Pi}(q) = n_i u_0^2 \sum_{\mathbf{k}} G_R(k)G_A(-k+q)$$

where we have denoted $G_R(k) \equiv G(\mathbf{k}, i\omega_r^+)$ and $G_A(k) \equiv G(\mathbf{k}, i\omega_r)$, implicitly assuming that ω_r^+ and ω_r are of opposite sign. Now if we look carefully at $\bar{\Pi}$, we see that it is identical to the particle hole bubble Π that we encountered when computing diffusive charge fluctuations in (11.32), excepting that in the hole line has been replaced by a particle line, and in so doing, we replace $\mathbf{k}+\mathbf{q} \to -\mathbf{k}+\mathbf{q}$

in the momentum of the propagator. However, thanks to time-reversal symmetry holds, this this does not change the value of the polarization bubble, and we conclude that

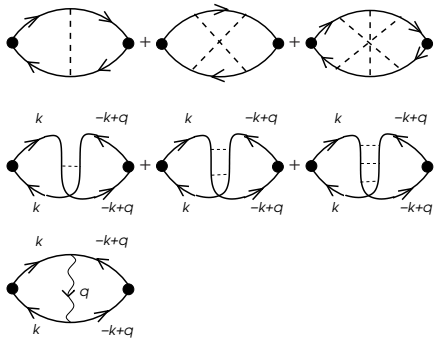
$$\tilde{\Pi}(q) = \left(1 - \nu_n\tau - Dq^2\tau + \ldots\right)$$

and thus

$$C(q) = n_i u_0^2 \frac{\tau^{-1}}{Dq^2 + |\nu_n|} = \frac{1}{2\pi N(0)\tau^2}\frac{1}{Dq^2 + |\nu_n|}$$

We shall redraw the maximally crossed contributions to the conductivity as follows

ΔQ_{ab} =



(11.43)

Written out explicitly, this gives

$$\begin{aligned}\Delta\sigma^{ab}(i\nu_n) &= \frac{\Delta Q^{ab}}{\nu_n} \\ &= \frac{2e^2T}{\nu_n}\sum_{k=(\mathbf{k},i\omega_r)\atop \mathbf{q}} v^a_{\mathbf{k}}v^b_{-\mathbf{k}+\mathbf{q}}\left[C(q)G^+(k)G^-(k)G^+(-k+q)G^-(-k+q) - \{i\nu_n \to 0\}\right]\end{aligned}$$

At this point, we can simplify the diagram by observing that to extract the most singular, long-distance effects of localization, we can ignore the smooth q dependence of the conduction electron lines. By setting $q = 0$ along the conduction lines, we decouple $\Delta\sigma$ into a product of two terms

$$\begin{aligned}\Delta\sigma^{ab}(i\nu_n) &= \frac{2e^2T}{\nu_n}\sum_{\mathbf{q}} C(q)\ \overbrace{\sum_k v^a_{\mathbf{k}}v^b_{-\mathbf{k}}}^{-\frac{\nu_n}{2\pi T}\frac{ne^2}{m}\delta^{ab}\int d\epsilon}\ \left[(G^+(k))^2(G^-(k))^2 - \{i\nu_n \to 0\}\right] \\ &= -\frac{ne^2}{m}\delta^{ab}\frac{1}{2\pi N(0)\tau^2}\int\frac{d^dq}{(2\pi)^d}\frac{1}{Dq^2 + |\nu_n|}\int\frac{d\epsilon}{2\pi}G^2_R(\epsilon)G^2_A(\epsilon) \qquad (11.44)\end{aligned}$$

The energy integral in the second term yields

$$\int\frac{d\epsilon}{2\pi}G^2_R(\epsilon)G^2_A(\epsilon) = 2\tau^3.$$

We need to consider the upper and lower bounds to the momentum integral. The upper bound is set by the condition that $Dq^2 = \tau^{-1}$, the elastic scattering rate. The lower bound is set either by the size of the system L, in which case $q = L^{-1}$, or by the *inelastic* scattering rate τ_i^{-1}. We may define

$$\tau_0^{-1} = \max(\frac{D}{L^2}, \tau_i^{-1})$$

as the inverse time-scale associated with the lower cutoff. The quantity

$$E_{th} = \hbar\frac{D}{L^2}$$

is called the "Thouless" energy, and corresponds to the energy scale associated with the phase-coherent diffusion of electrons from one side of the sample, to the other. In an ultra-pure, or small system, it is this scale that provides the infra-red cut-off to localization effects. We may then write

$$\Delta\sigma^{ab}(\nu) = -\delta^{ab}\left(\frac{ne^2\tau}{m}\right)\frac{1}{2\pi N(0)}\int_{(D\tau_o)^{-1/2}}^{(D\tau)^{-1/2}}\frac{d^dq}{(2\pi)^d}\frac{1}{Dq^2 - i\nu} \qquad (11.45)$$

If we apply a sudden pulse of electric field $E = E_0\delta(t)$, giving rise to a white noise field spectrum, $E(\nu) = E_0$, the current induced by localization effects has a frequency spectrum

$$j(\nu) = \Delta\sigma(\nu)E(\nu) = \Delta\sigma(\nu)E_0 \propto \int_{(D\tau_0)^{-1/2}}^{(D\tau)^{-1/2}}\frac{d^dq}{(2\pi)^d}\frac{1}{Dq^2 - i\nu}$$

In highly phase-coherent systems, the characteristic time scale of the localization back-scattering response in the current pulse is given by $t \sim D/L^2$ which we recongnize as the time for electrons to diffuse across the entire sample. This is a kind of backscattering "echo" produced by the phase-coherent diffusion of electrons along time-reversed paths that cross the entire sample. The momentum integral in $\Delta\sigma$ is strongly dependent on dimensionality. in three and higher dimensions, this term is finite, so that the weak-localization effects are a perturbation to the Drude conductivity. However, if the dimension $d \le 2$, this integral becomes divergent, and in a non-interacting system, it is cut off only by the frequency, or the finite size L of the system. In two dimensions,

$$\int_{(D\tau_o)^{-1/2}}^{(D\tau)^{-1/2}}\frac{d^dq}{(2\pi)^d}\frac{1}{Dq^2 - i\nu} = \frac{1}{4\pi D}\ln(\frac{\tau}{\tau_0})$$

giving rise to a localization correction to the static conductivity that is

$$\Delta\sigma = -\left(\frac{ne^2\tau}{m}\right)\frac{1}{8\pi^2N(0)D}\ln(\frac{\tau_0}{\tau}) \qquad (11.46)$$

Replacing $n\tau/m \to 2N(0)D$, we obtain

$$\Delta\sigma = -\left(\frac{e^2}{2\pi^2}\right)\ln(\frac{\tau}{\tau_0}) \to -\frac{1}{2\pi^2}\left(\frac{e^2}{\hbar}\right)\ln(\frac{\tau_0}{\tau}) \tag{11.47}$$

where we have restored $\hbar$ into the expression. The quantity $g_0 = \frac{e^2}{\hbar} \sim \frac{1}{10}(k\Omega)^{-1}$ is known as the universal conductance.

There are a number of interesting consequences of these results

- By replacing $2\pi N(0)D = \frac{1}{2}k_F l$, the total conductivity can be written

$$\sigma = \sigma_0\left[1 - \frac{1}{2\pi k_F l}\ln(\frac{\tau_0}{\tau})\right] \tag{11.48}$$

  We see that the quantum-interference correction to the conductivity is of order $O(1/(k_F l))$, justifying their neglect in our earlier calculations.

- If we consider the case where inelastic scattering is negligible, the localization correction to the conductivity in two dimensions is

$$\begin{aligned}\sigma &= \sigma_0\left[1 - \frac{1}{2\pi k_F l}\ln(\frac{1}{E_{Th}\tau})\right] \\ &\sim \sigma_0\left[1 - \frac{1}{\pi k_F l}\ln(\frac{L}{l})\right]\end{aligned} \tag{11.49}$$

  so that the conductivity drops gradually to zero as the size of the sample increases. The conductivity becomes of order $\frac{e^2}{\hbar}$ at the "localization length"

$$L_c \sim l e^{k_F l}$$

  independently of the strength of the interaction. In two dimensions, resistivity and resistance have the same dimension, so we expect that when the size of the system is equal to the localization length, the resistivity is always of order $10k\Omega$! At longer length-scales, the material evolves into insulator.

- The weak localization corrections are not divergent for dimensions greater than 2, but become much stronger in dimensions below $d = 2$. It was this observation that led the the "Gang of Four", Abrahams, Anderson, Licciardello and Ramakrishnan, to propose the scaling theory for localization, in which $d_c = 2$ is the critical dimensionality.

We shall end this section by making a brief remark about the scaling theory of localization. Stimulated by the results in two dimensions, and earlier work on one dimensional wires, by Thouless, Abrahams et al. were led to propose that in any dimension, conductance, or inverse resistance, $G = 1/R$ could always be normalized to form a dimensionless parameter

$$g(L) = \frac{G(L)}{\frac{e^2}{\hbar}}$$

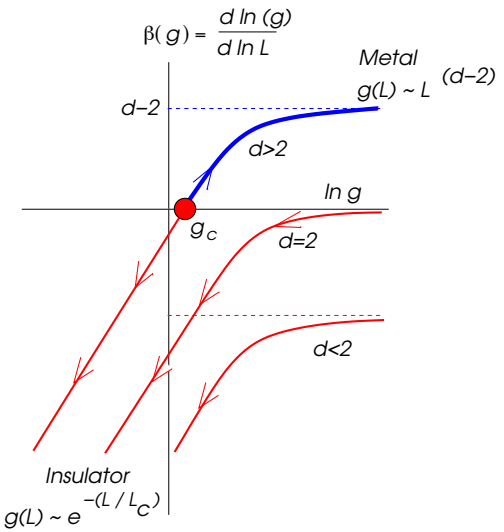


Figure 11.6: The scaling function $\beta(g)$ deduced by Abrahams et al. for a non-interacting metal. For $d > 2$ there is critical conductance g_c which gives rise to a disorder-driven metal-insulator transition. In $d \le 2$, disorder always gives rise to localization and the formation of an insulator.

which satisfies a one-parameter scaling equation

$$\frac{d\ln g(L)}{d\ln L} = \beta(g)$$

When this quantity is large, we may use the Drude model, so that $g(L) = \frac{ne^2\tau}{m}L^{d-2}$, and

$$\beta(g) = (d-2), \qquad (g \to \infty)$$

is independent of g. When the conductance was small $g \to 0$, on scales longer than the localization length L_c, they argued that $g(L)$ would decay exponentially $g(L) \sim e^{-L/L_c}$, so that for small conductance,

$$\beta(g) \sim -\ln g, \qquad (g \to 0)$$

By connecting up these two asymptotic limits, Abrahams et al reasoned that the beta function for conductance would take the form shown in Fig. 11.6. In dimensions $d \le 2$, the $\beta(g)$ is always negative, so the conductance always scales to zero and electrons are always localized. However in dimensions $d > 2$, there is a disorder-driven metal-insulator transition at the critical conductance

$g = g_c$. As the amount of disorder is increased, when the short-distance conductance g passes below g_c, the material becomes an insulator in the thermodynamic limit. These heuristic arguments stimulated the development of a whole new field of research into the collective effects of disorder on conductors, and the basic results of the scaling theory of localization are well-established in metals where the effects of interactions between electrons are negligible. Interest in this field continues actively today, with the surprise discovery in the late 1990s that two dimensional electron gases formed within heterojunctions appear to exhibit a metal insulator transition - a result that confounds the one-parameter scaling theory, and is thought in some circles to result from electron-electron interaction effects.

11.6 Exercises

1. (Alternative derivation of the electrical conductivity.)

   In our treatment of the electrical conductivity, we derived

$$\sigma^{ab}(i\nu_n) = e^2 \frac{T}{\nu_n} \sum_{\mathbf{k}, i\omega_r} v^a_{\mathbf{k}} v^b_{\mathbf{k}} \left[G(\mathbf{k}, i\omega_r + i\nu_n) G(\mathbf{k}, i\omega_r) - G(\mathbf{k}, i\omega_r)^2 \right]$$

   This integral was carried out by first integrating over momentum, then integrating over frequency. This techique is hard to generalize and it is often more convenient to integrate the expression in the opposite order. This is the topic of this question. Consider the case where

$$G(\mathbf{k}, i\omega_r) = \frac{1}{i\omega_r - \epsilon_{\mathbf{k}} - \Sigma(i\omega_r)}$$

   and $\Sigma(i\omega_r)$ is any momentum-independent self-energy.

   (a) By rewriting the momentum integral as an integral over kinetic energy ϵ and, angle show that the conductivity can be rewritten as $\sigma^{ab}(i\nu_n) = \delta^{ab}\sigma(i\nu_n)$, where

$$\sigma(i\omega_n) = \frac{ne^2}{m} \frac{1}{\nu_n} \int_{-\infty}^{\infty} d\epsilon \; T \sum_{i\omega_r} \left[G(\epsilon, i\omega_r + i\nu_n) G(\epsilon, i\omega_r) - G(\epsilon, i\omega_r)^2 \right].$$

   and

$$G(\epsilon, z) \equiv \frac{1}{z - \epsilon - \Sigma(z)}$$

   (b) Carry out the Matsubara sum in the above expression to obtain

$$\sigma(i\omega_n) = \frac{ne^2}{m} \frac{1}{\nu_n} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \int_{-\infty}^{\infty} d\epsilon f(\omega) \left[G(\epsilon, \omega + i\nu_n) + G(\epsilon, \omega - i\nu_n) \right] A(\epsilon, \omega),$$

   where $A(\epsilon, \omega) = ImG(\epsilon, \omega - i\delta)$. (*Hint - replace* $T\sum_n \to -\int \frac{dz}{2\pi i} f(z)$, *and notice that while* $G(\epsilon, z)$ *has a branch cut along* $z = \omega$ *with discontinuity given by* $G(\epsilon, \omega - i\delta) - G(\epsilon, \omega + i\delta) = 2iA(\epsilon, \omega)$, *while while* $G(\epsilon, z + i\nu_n)$ *has a similar branch cut along* $z = \omega - i\nu_n$. *Wrap the contour around these branch cuts and evaluate the result*).

   (c) Carry out the energy integral in the above expression to obtain

$$\sigma(i\omega_n) = \frac{ne^2}{m} \frac{1}{\nu_n} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} f(\omega) \times \left[\frac{1}{i\nu_n - (\Sigma(\omega + i\nu_n) - \Sigma(\omega - i\delta))} - \frac{1}{i\nu_n - (\Sigma(\omega + i\delta) - \Sigma(\omega - i\nu_n))} \right]. \quad (11.50)$$

   (d) Carry out the analytic continuation in the above expression to finally obtain

$$\sigma(\nu + i\delta) = \frac{ne^2}{m} \int_{-\infty}^{\infty} d\omega \left[\frac{f(\omega - \nu/2) - f(\omega + \nu/2)}{\nu} \right] \times \frac{1}{-i\nu + i(\Sigma(\omega + \nu/2 + i\delta) - \Sigma(\omega - \nu/2 - i\delta))}. \quad (11.51)$$

   (e) Show that your expression for the optical conductivity can be rewritten in the form

$$\sigma(\nu + i\delta) = \frac{ne^2}{m} \int_{-\infty}^{\infty} d\omega \left[\frac{f(\omega - \nu/2) - f(\omega + \nu/2)}{\nu} \right] \frac{1}{\tau^{-1}(\omega, \nu) - i\nu Z(\omega, \nu)}. \quad (11.52)$$

   where

$$\tau^{-1}(\omega, \nu) = \mathrm{Im}\left[\Sigma(\omega - nu/2 - i\delta) + \Sigma(\omega + \nu/2 - i\delta)\right] \quad (11.53)$$

   is the average of the scattering rate at frequencies $\omega \pm \nu/2$ and

$$Z^{-1}(\omega, \nu) - 1 = -\frac{1}{\nu} \mathrm{Re}\left[\Sigma(\omega - \nu/2) - \Sigma(\omega + \nu/2)\right]$$

   is a kind of "wavefunction renormalization".

   (f) Show that if the ω dependence of Z and τ^{-1} can be neglected, one arrives at the phenomenological form

$$\sigma(\nu) = \frac{ne^2}{m} \left[\frac{1}{\tau^{-1}(\nu) - i\nu Z^{-1}(\nu)} \right]$$

   This form is often used to analyze optical spectra.

   (g) Show that the zero temperature conductivity is given by the thermal average

$$\sigma(\nu + i\delta) = \frac{ne^2\tau}{m} \quad (11.54)$$

   where $\tau^{-1} = 2Im\Sigma(0 - i\delta)$.

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[1] F. London, *Superfluids*, Dover Publications, New York, 1961-64.

Chapter 12

Phase Transitions and broken symmetry

12.1 Order parameter concept

The idea that phase transitions involve the development of an order parameter which lowers, or "breaks" the symmetry is one of the most beautiful ideas of many body physics. In this chapter, we introduce this new concept, which plays a central role in our understanding of the way complex systems transform themselves into new states of matter at low temperatures.

Landau introduced the order parameter concept in 1937[1] as a means to quantify the dramatic transformation of matter at a phase transition. Examples of such transformations abound: a snowflake forms when water freezes; iron becomes magnetic when electron spins align into a single direction; superfluidity and superconductivity develop when quantum fluids are cooled and bosons or pairs of fermions condense into a single quantum state with a well-defined phase. Phase transitions can even take place in very fabric of space, and there is very good evidence that we are living in a broken symmetry universe, which underwent one, or more phase transitions which broke the degeneracy between the fundamental forces[2], shortly after the big bang. Indeed, when the sun shines on our faces, we are experiencing the consequences of this broken symmetry. Remarkably, while the microscopic physics of each case is different, they are unified by a single concept.

Landau's theory associates each phase transition with the development of an "order parameter" ψ once the temperature drops below the transition temperature T_c:

$$|\psi| = \begin{cases} 0 & (T > T_c) \\ |\psi_0| > 0 & (T < T_c) \end{cases}$$

The order parameter can be a real or complex number, a vector or a spinor that can, in general, be related to an n-component real vector $\psi(x) = (\psi_1, \psi_2 \ldots \psi_n)$. For example:

Order parameter	Realization	Microscopic origin
$m = \psi_1$	Ising ferromagnet	$\langle \hat{\sigma}_z \rangle$
$\psi = \psi_1 + i\psi_2$	Superfluid, Superconductor	$\langle \hat{\psi}_B \rangle$, $\langle \hat{\psi}_\uparrow \hat{\psi}_\downarrow \rangle$
$\vec{M} = (\psi_1, \psi_2, \psi_3)$	Heisenberg Ferromagnet	$\langle \vec{\sigma} \rangle$
$\Phi = \begin{pmatrix} \psi_1 + i\psi_2 \\ \psi_3 + i\psi_4 \end{pmatrix}$	Higg's Field	$\begin{pmatrix} \langle \hat{\phi}_+ \rangle \\ \langle \hat{\phi}_- \rangle \end{pmatrix}$

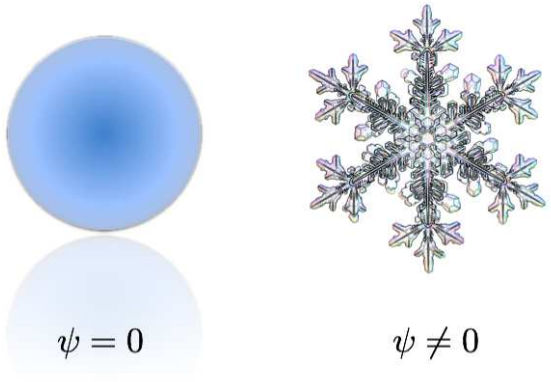

Figure 12.1: "Broken symmetry". The development of crystalline order within a spherical water-droplet leads to the formation of a snowflake, reducing the symmetry from spherical symmetry, to six-fold symmetry. (Snowflake picture reproduced with permission from K. G. Librrecht.)

Microscopically, each order parameter is directly related to the expectation value of a quantum operator. Thus, in an Ising ferromagnet "$m = \langle \sigma_z(x) \rangle$" is the expectation value of the spin density along a particular anisotropic axis, while in a Heisenberg ferromagnet, the magnetization can point in any direction, so that the order parameter is a vector pointing in the direction of the spin density $\vec{m} = \langle \vec{\sigma}(x) \rangle$. In a superconductor or superfluid, the order parameter is a complex number related to the expectation value a bosonic field in the condensate.

The emergence of an order parameter often has dramatic macroscopic consequences in a material. In zero gravity, water droplets are perfectly spherical, yet if cooled through their freezing

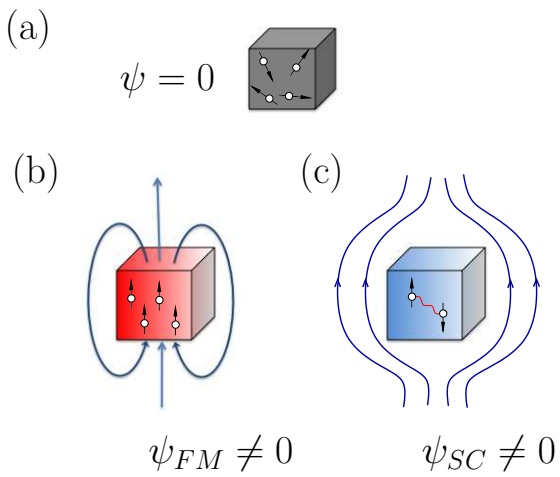

Figure 12.2: (a) In a normal metal, there is no long-range order. (b) Below the Curie temperature T_c of a ferromagnet, electron spins align to develop a ferromagnetic order parameter. The resulting metal has a finite magnetic moment. (c) Below the transitition temperature of a superconductor, electrons pair together to develop a superconducting order parameter. The resulting metal exhibits the Meissner effect, excluding magnetic fields from its interior.

point they form crystals of ice with the classic six-fold symmetry of a snowflake. We say that the symmetry of the water has "broken the symmetry", because the symmetry of the ice crystal no longer enjoys the continuous rotational symmetry of the original water droplet. Equally dramatic effects occur within quantum fluids. Thus, when a metal develops a ferromagnetic order parameter, it spontaneously develops an internal magnetic field. By contrast, when a metal develops superconducting order, it behaves as a perfect diamagnet, and will spontaneously expel magnetic fields from its interior even when cooled in a magnetic field, giving rise to what is called the "Meissner effect".

Part of the beauty of Landau theory, is that the precise microscopic expression for the order parameter is not required to development a theory of the macroscopic consequences of broken symmetry. The Ginzburg-Landau theory of superconductivity pre-dated the microscopic theory by seven years. Landau theory provides a "coarse grained" description of the properties of matter. In general, the order parameter description is good on length scales larger than

$$\xi_0 = \text{"coherence length"}. \tag{12.1}$$

On length-scales longer than coherence length, the internal structure of the order parameter is irrelevant and it behaves as a smootly varying function that has forgotten about its microscopic origins. However, physics on scales smaller than ξ_0 requires a microscopic description. For example, in a superconductor, the coherence length is a measure of the size of a Cooper pair - a number that can be hundred or thousands of atom spacings, while in superfluid $He-4$, the coherence length is basically an atom spacing.

12.2 Landau Theory

12.2.1 Field cooling and the development of order

The basic idea of Landau theory, is to write the free energy as a function $F[\psi]$ of the order parameter. To keep things simple, we will begin our discussion with the simpest case when ψ is a one-component Ising order parameter representing, for example, the magnetization of an Ising Ferromagnet. We begin by considering the meaning of an order parameter, and the relationship of the the free energy to the microscopic physics.

We can always induce the order parameter to develop by cooling in the presence of an external field h that couples to the order parameter. In general, the inverse dependence of the field on the order parameter, $h[\psi]$ will be highly non-linear, but once we know it, we can convert the dependence of the energy on h to a function of ψ. Broken symmetry develops if ψ remains finite once the external field is removed.

Mathematically, an external field introduces a "source term" into the microscopic Hamiltonian:

$$H \to H - h\int d^3x\hat{\psi}(x).$$

The field h that couples linearly to the order parameter is called the conjugate field. For an magnet, where $\psi \equiv M$ is the magnetization, $h \equiv B$ is the external magnetic field. For a ferro-electric, where $\psi \equiv P$ is the electric polarization, the conjugate field $h \equiv E$ is the external electric field. For many classes of order parameter, such as the pair density of a superconductor, or the staggered magnetization of an antiferromagnet, although there is no naturally occuring external field that couples linearly to the order parameter, but the idea of a conjugate field is still a very useful concept.

The free energy of the system in the presence of an external field is a Gibb's free energy which takes account of the coupling to the field $\mathcal{G}[h] = F[\psi] - V\psi h$. $\mathcal{G}[h]$ is given by

$$\mathcal{G}[h] = -k_BT\ln(Z[h]) = -k_BT\ln\left(\mathrm{Tr}\left[e^{-\beta(\hat{H}-h\int\hat{\psi}d^3x)}\right]\right) \tag{12.2}$$

where the partition function $Z[h]$ involves the trace over the many body system. If we differentiate (12.2) with respect to h we recover the expectation value of the induced order parameter $\psi[h] = \langle\hat{\psi}\rangle$

$$\psi(h,V) = \frac{1}{Z[h]}\mathrm{Tr}\left[e^{-\beta(H-h\int\psi d^3x)}\hat{\psi}(x)\right] = -\frac{1}{V}\frac{\partial\mathcal{G}[h]}{\partial h}, \tag{12.3}$$

It follows that $-\delta\mathcal{G} = \psi V\delta h$.

In a finite system, the order parameter will generally disappear once we remove the finite field. For example, if we take a molecular spin cluster and field-cool it below its bulk Curie temperature it will develop a finite magnetization. However, once we remove the external field, thermal fluctuations will generate domains with reversed order. Each time a domain wall crosses the system, the magnetization reverses, so that on long enough time scales, the magnetization will average to zero. But as the size of the system grows beyond the nano-scale, two things will happen - first infinitesimal fields will prevent the thermal excitation of macroscopic domains - and second - even in a truly zero field, the probability to form these large domains becomes astronomically small. (See example Ex. 12.2.1) In this way, broken symmetry "freezes into" the system and becomes stable in the thermodynamic limit.

From this line of reasoning, it becomes clear that the development of a thermally stable order parameter requires that we take the thermodynamic limit $V \to \infty$ before we remove the external field. When we "field cool" an infinitely large system below a second-order phase transition, the order parameter remains after the external field is removed. The equilibrium order parameter is then defined as

$$\psi = \lim_{h\to 0}\lim_{V\to\infty} \psi(h, V).$$

To obtain the Landau function, $F[\psi]$, must write $\mathcal{G}[h]$ in terms of ψ and then,

$$F[\psi] = \mathcal{G}[h] + Vh\psi = \mathcal{G}[h] - h\frac{\partial \mathcal{G}[h]}{\partial h}.$$

This expression for $F[\psi]$ is a Legendre transformation of $\mathcal{G}[h]$. Since $\delta\mathcal{G} = -V\psi\delta h$, $\delta F = \delta\mathcal{G} + V\delta(h\psi) = Vh\delta\psi$, so the inverse transformation is $h = V^{-1}\frac{\partial F}{\partial \psi}$. If $h = 0$, then

$$hV = \frac{\partial F}{\partial \psi} = 0$$

which states the intuitively obvious fact that when $h = 0$, the equilibrium value of ψ is determined by a stationary point of $F[\psi]$.

Example 12.1: Consider a cubic nanomagnet of $N = L^3$ Ising spins interacting via a nearest neighbor ferromagnetic interaction of strength J. Suppose the dynamics can be approximated by Monte Carlo dynamics, in which each spin is "updated" after a a time τ_0. At $T = 2J$, (the bulk $T_c = 4.52J$) estimate the time, in units of τ_0 required to form a domain that will cross the entire sample. If $\tau_0 = 1ns$, estimate the minimum size L for the decay time of the total magnetization to become comparable with the time span of a Ph. D. degree.

Solution: To form a domain wall of area $A \sim L^2$ costs an free energy $\Delta F \sim 2JL^2$, occuring with probability $p \sim e^{-(\Delta F/T)}$. The time required for formation may be estimated to be

$$\tau \sim \tau_0 p^{-1} \sim \tau_0 e^{2JL^2/T}.$$

where the most important aspect of the estimate, is that the exponent grows with L^2. Our naive estimate does not take into account the configurational entropy (the number of ways of

arranging a domain wall), but it will give a rough idea of the required size. Putting $\tau_0 \sim 10^{-9}s$ and $\tau = 5y \sim 10^8$s for a typical Ph. D, this requires $\tau/\tau_0 = 10^{19} \sim e^{40}$, thus $L \sim \sqrt{40} \sim 6$. Already by about $L^3 = 40^{3/2} \sim 250$ spins the time for the magnetization to decay is of the order of years. By $N \sim 500$, this same timescale has stretched to the age of the universe.

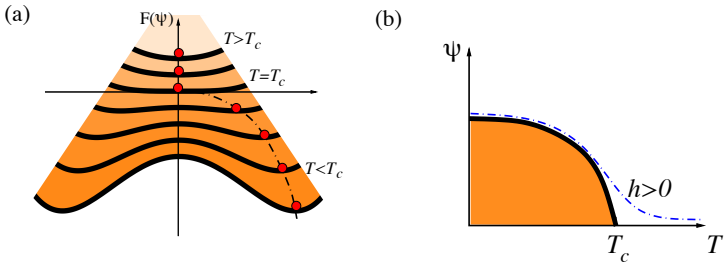

Figure 12.3: (a) The Landau free energy $F(\psi)$ as a function of temperature for an Ising order parameter. Curves are displaced vertically for clarity. (b) Order parameter ψ as a function of temperature for a finite field $h > 0$ and an infinitesimal field $h = 0^+$.

12.2.2 The Landau Free energy

Landau theory concentrates on the region of small ψ, audaciously expanding the free energy of the many body system as a simple polynomial:

$$f_L[\psi] = \frac{1}{V}F[\psi] = \frac{r}{2}\psi^2 + \frac{u}{4}\psi^4. \tag{12.4}$$

- The Landau free energy describes the leading dependence of the total free energy on ψ. The full free energy is given by $f_{tot} = f_n(T) + f[\psi] + O[\psi^4]$, where f_n is the energy of the "normal" state without long range order.
- For an Ising order parameter, both the Hamiltonian and the free energy are an even function of ψ: $H[\psi] = H[-\psi]$. We say that the system possesses a "global Z_2 symmetry", because the Hamiltonian is invariant under transformations of the Z_2 group that takes $\psi \to \pm\psi$.

Provided r and u are greater than zero, the minimum of $f_L[\psi]$ lies at $\psi = 0$. Landau theory assumes that the phase transition temperuture, r changes sign, so that

$$r = a(T - T_c)$$

as illustrated in Fig. 12.3 (a). The minimum of the free energy occurs when

$$\frac{df}{d\psi} = 0 = r\psi + u\psi^3 \Rightarrow \psi = \begin{cases} 0 & (T > T_c) \\ \pm\sqrt{\frac{a(T_c - T)}{u}} & (T < T_c) \end{cases} \tag{12.5}$$

so that for $T < T_c$, there are two minima of the free energy function (Fig. 12.3 (a)). Note that:

- if we cool the system in a tiny external field, the sign of the order parameter reflects the sign of the field (Fig. 12.3 (b)):

$$\psi = \mathrm{sgn}(h)\sqrt{\frac{a(T_c - T)}{u}}, \qquad (T < T_c). \tag{12.6}$$

  This branch-cut along the temperature axis of the phase diagram, is an example of a first-order phase boundary. The point $T = T_c$, $h = 0$ where the line ends is a **"critical point"**.

- If $u < 0$ the free energy becomes unbounded below. To cure this problem, the Landau free energy must be expanded to sixth order in ψ:

$$f[\psi] = \frac{1}{V}F[\psi] = \frac{r}{2}\psi^2 + \frac{u}{4}\psi^4 + \frac{u_6}{6}\psi^6$$

  When $u < 0$ the free energy curve develops three minima and the phase transition becomes first order; the special point at $r = h = u = 0$ is a convergence of three critical points called a **tri-critical point** (see exercise 3).

12.2.3 Singularities at the critical point.

At a second order phase transition, the second derivatives of the Free energy develop singularities. If we plug (12.6) back into the Free energy $f_L[\psi]$ (12.4), we find that

$$f_L = \begin{cases} 0 & (T > T_c) \\ -\frac{a^2}{4u}(T_c - T)^2 & (T < T_c) \end{cases}$$

In this way, the free energy and the entropy $S = -\frac{\partial F}{\partial T}$ are continuous at the phase transition, but the specific heat

$$C_V = -T\frac{\partial^2 F}{\partial T^2} = C_0(T) + \begin{cases} 0 & (T > T_c) \\ \frac{a^2 T}{2u} & (T < T_c) \end{cases} \tag{12.7}$$

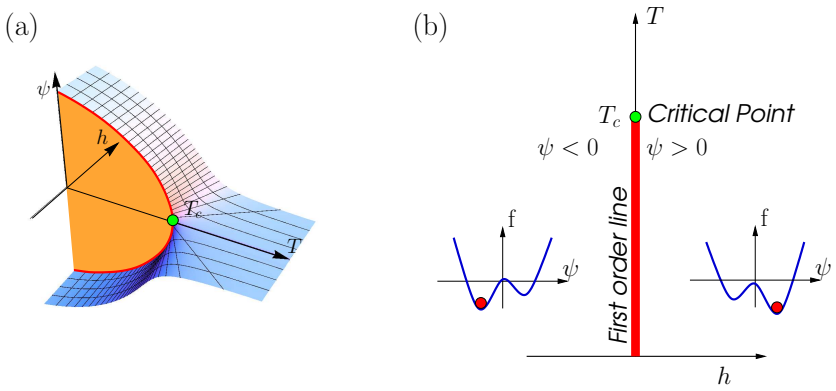

Figure 12.4: Phase diagram in an applied field. A first order line stretches along the zero field axis, $h = 0$ up to the critical point. The equilibrium order parameter changes sign when this phase boundary is crossed. (a) Three dimensional plot showing discontinuity in order parameter as a function of field ψ. (b) Two dimensional phase boundary showing first order line.

where C_0 is the background component of the specific heat not associated with the ordering process. We see that C_V "jumps" by an amount

$$\Delta C_V = \frac{a^2 T_c}{2u}$$

below the transition. The jump size ΔC_V has the dimensions of entropy per unit volume, and sets a characteristic size of the entropy lost per unit volume once long-range order sets in.

At a second-order transition, matter also becomes infinitely susceptible to the applied field h, as signalled by a divergence in susceptibility $\chi = \frac{\partial \psi}{\partial h}$. To see this in Landau theory, let us introduce a field by replacing

$$f(\psi) \to f(\psi) - h\psi = \frac{r}{2}\psi^2 + \frac{u}{4}\psi^4 - h\psi \tag{12.8}$$

A finite field $h > 0$ has the effect of "tipping" the free energy contour to the right, preferentially lowering the energy of the right-hand minimum, as illustrated in Fig. (12.4). For $h \neq 0$, equilibrium requires $\partial f/\partial\psi = r\psi + u\psi^3 - h = 0$, which we can solve for $r = \frac{h}{\psi} - 4u\psi^2$. Above and below T_c, we can solve for ψ by linearizing $\psi[h] = \delta\psi + \psi_0$ around the $h = 0$ value given in (12.6), to obtain $\delta\psi = \chi(T)h + O(h^3)$, (See Fig. 12.3(b)) where

$$\chi(T) = \frac{d\psi}{dh} = \frac{1}{a|T - T_c|} \times \begin{cases} 1 & (T > T_c) \\ \frac{1}{2} & (T < T_c) \end{cases} \tag{12.9}$$

describes the divergence of the "susceptibility" at the critical point. When we are actually at the critical point ($r = 0$), the induced order parameter is a non-linear function of field,

$$\psi = \left(\frac{h}{u}\right)^{1/3} \qquad (T = T_c) \tag{12.10}$$

The divergence of the susceptibility at the critical point means that if cool through the critical point in the absence of a field, the tiniest stray field will produce a huge effect, tipping the system into either an up or down state. Once this happens, we say that the system has *"spontaneously broken the Z_2 inversion symmetry"* of the original Hamiltonian.

The singular powerlaw dependences of the order parameter, specific heat and susceptibility near a second order transition described by Landau theory are preserved at real second-order phase transitions, but the critical exponents are changed by the effects of spatial fluctuations of the order parameter. In general, we write

$$\begin{aligned} C_V &\propto (|T - T_c|)^{-\alpha} && \text{(Specific heat)}, \\ \psi &\propto \begin{cases} (T_c - T)^{\beta} \\ h^{\frac{1}{\delta}} \end{cases} && \text{(Order parameter)}, \\ \chi &\propto (T - T_c)^{-\gamma} && \text{(Susceptibility)}, \end{aligned} \tag{12.11}$$

which Landau theory estimates as $\alpha = 0, \beta = 1/2, \delta = 3$ and $\gamma = 1$. Remarkably, this simple prediction of Landau theory continues to hold once the full-fledged effects of order parameter fluctuations are included, and still more remarkably, the exponents that emerge are found to be universal for each class of phase transition, independently of the microscopic physics[3].

12.2.4 Broken Continuous symmetries : the Mexican Hat Potential

We now take the leap from a one, to an n-component order parameter. We shall be particularly interested in a particularly important class of multi-component order in which the underlying physics involves a continous symmetry that is broken by the phase transition. In this case, the *n−component* order parameter $\vec{\psi} = (\psi_1 \ldots \psi_n)$ acquires both magnitude and direction, and the discrete Z_2 inversion symmetry of the Ising model is now replaced by a continuous "$O(N)$" rotational symmetry. At a phase transition the breaking of such continous symmetries has remarkable consequences.

The $O(N)$ symmetric Landau theory is simply constructed by replacing $\psi^2 \to |\psi|^2 = (\psi_1^2 + \ldots \psi_n^2) = \vec{\psi} \cdot \vec{\psi}$, taking the form

$$f_L[\vec{\psi}] = \frac{r}{2}(\vec{\psi} \cdot \vec{\psi}) + \frac{u}{4}[(\vec{\psi} \cdot \vec{\psi})]^2, \qquad O(N) \text{ invariant Landau theory}$$

where as before $r = a(T - T_c)$. This Landau function is invariant under $O(N)$ rotations $\vec{\psi} \to R\vec{\psi}$ that preserve the magnitude of the order parameter. Such symmetries do not occur by accident, but owe their origin to conservation laws which protect them in both the microscopic Hamiltonian and

the macroscopic Landau theory. For example, in a Heisenberg magnet, the corresponding Landau theory has $O(3)$ symmetry associated with the underlying conservation of the total spin magnetization.

Once $T < T_c$, the order parameter acquires a definite magnitude and direction given by

$$\vec{\psi} = \sqrt{\frac{|r|}{u}}\hat{n}$$

where $\hat{n}$ is a unit (n-component) vector. By acquiring a definite direction, the order parameter breaks the $O(N)$ symmetry. In a magnet, this would correspond to the spontaneous development of a uniform magnetization. In a superconductor or superfluid, it corresponds to the development of a macroscopic phase.

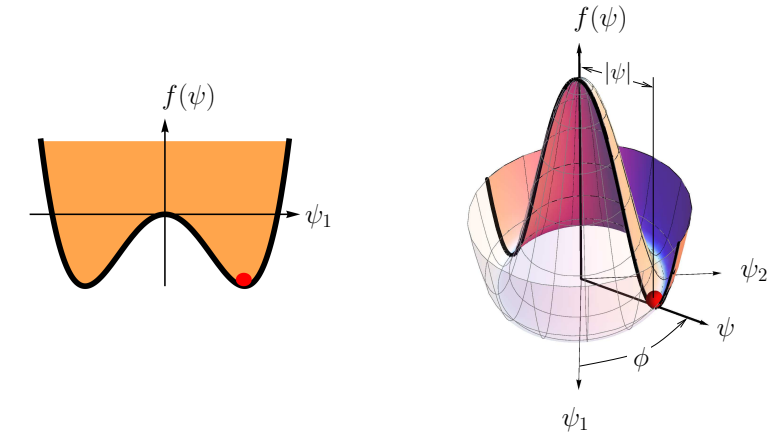

Figure 12.5: Dependence of Free energy on order parameter for (a) an Ising order parameter $\psi = \psi_1$, showing two degenerate minima and (b) complex order parameter $\psi = \psi_1 + i\psi_2 = |\psi|e^{i\phi}$, where the the Landau free energy forms a "Mexican Hat Potential" in which the free energy minimum forms a rim of degenerate states with energy that is independent of the phase ϕ of the uniform order parameter.

A particularly important example of a broken continuous symmetry occurs in superfluids and superconductors, where the the order parameter is a single complex order parameter composed from

two real order parameters $\psi = \psi_1 + i\psi_2 = |\psi|e^{i\phi}$. In this case, the Landau free energy takes the form[1]

$$\begin{aligned} f[\psi] &= r(\psi^*\psi) + \frac{u}{2}(\psi^*\psi)^2, \qquad U(1) \text{ invariant Landau theory} \\ \psi &\equiv \psi_1 + i\psi_2 \equiv |\psi|e^{i\phi}. \end{aligned} \tag{12.12}$$

Fig. (12.5) shows the Landau free energy as a function of ψ, where the magnitude of the order parameter $|\psi|$ is represented in polar co-ordinates. The free energy surface displays a striking rotational invariance, associated with the fact that the free energy is independent of the global phase of the order parameter

$$f[\psi] = f[e^{i\alpha}\psi]. \qquad U(1) \text{ gauge invariance}$$

This is a direct consequence of the global $U(1)$ invariance of the particle fields that have condensed to develop the complex order parameter. For $T < T_c$, the negative curvature of the free energy surface at $\psi = 0$ causes the free energy surface to develops the profile of a "Mexican Hat", with a continuous rim of equivalent minima where

$$\psi = \sqrt{\frac{|r|}{u}}e^{i\phi}$$

The appearance of a well-defined phase breaks the continuous $U(1)$ symmetry.

The "Mexican hat" potential illustrates a special property of phases with broken continuous symmetry: it becomes possible to continuously rotate the order parameter from one broken symmetry state to another. Notice however, that if the order parameter is to maintain a well-defined phase, or direction then it is clear that there must be an energy cost for deforming or "twisting" the direction of the order parameter. This rigidity is an essential component of broken continuous symmetry. In superfluids, the emergence of a well-defined phase associated with the order parameter is intimately related to persistent currents, or superflow. We shall shortly see that when we "twist" the phase, a superflow develops.

$$\vec{j} \propto \vec{\nabla}\phi.$$

To describe this rigidity, we need to take the next step, introducing a term into energy functional that keeps track of the energy cost of a non-uniform order parameter. This leads us onto Landau Ginzburg theory.

12.3 Ginzburg Landau theory I: Ising order

Landau theory describes the energy cost of a uniform order parameter: a more general theory needs to account for inhomogenious order parameters in which the amplitude varies or the direction of the order parameter is "twisted". This development of Landau theory is called "Ginzburg Landau"

[1] For complex fields, it is more convenient to work without the factor of 1/2 in front of the quadratic terms. To keep the numerology simple, the interaction term is also multiplied by two.

theory[2], after Ginzburg and Landau[5], who developed this formalism as part of their macroscopic theory of superconductivity. We will begin our discussion of Landau Ginzburg theory with the simplest case a one-component "Ising" order parameter.

Ginzburg Landau theory[5] introduces an addition energy cost $\delta f \propto |\nabla\psi|^2$ associated with gradients in the order parameter: $f_{GL}[\psi, \nabla\psi] = \frac{s}{2}|\nabla\psi|^2 + f_L[\psi(x)]$. For a single, Ising order parameter, the Free energy (in "d" dimensions) is given by

$$\begin{aligned} F_{GL}[\psi] &= \int d^d x f_{GL}[\psi(x), \nabla\psi(x), h(x)] \\ f_{GL}[\psi, \nabla\psi, h] &= \frac{s}{2}(\nabla\psi)^2 + \frac{r}{2}\psi^2 + \frac{u}{4}\psi^4 - h\psi \end{aligned} \tag{12.13}$$

Ginzburg Landau Free energy: one component order

There are two points to be made here:

- Ginzburg Landau (GL) theory is only valid near the critical point, where the order parameter is small enough to permit a leading order expansion.
- Dimensional analysis shows that $[c]/[r] = L^2$ has the dimensions of length-squared. The new length-scale introduced by the gradient term, called the "correlation length"

$$\xi(T) = \sqrt{\frac{s}{|r(T)|}} = \xi_0 \left|1 - \frac{T}{T_c}\right|^{-\frac{1}{2}} \qquad \text{correlation length} \tag{12.14}$$

sets the characteristic length-scale of order-parameter fluctuations, where

$$\xi_0 = \xi(T = 0) = \sqrt{\frac{s}{aT_c}} \qquad \text{coherence length}$$

is a measure of the microscopic coherence length. Near the transition, $\xi(T)$ diverges, but far from the transition, it becomes comparable with the coherence length.

The traditional use of Ginzburg Landau theory, is as a as a *variational principle*, using the condition of stationarity $\delta F/\delta\psi = 0$ to determine non-equilibrium configurations of the order parameter. Landau Ginzburg theory is also the starting point for a more general analysis of thermal fluctuations around the mean-field theory. We shall return at the end of this chapter.

12.3.1 Non-uniform solutions of Ginzburg Landau theory

There are two kinds of non-uniform solutions we will consider:

[2] The idea of using a gradient expansion of the free energy first appears in print in the work of Ginzburg and Landau. However, germs of this theory are contained in the work of Ornstein and Zernicke, who in 1914 developed a theory to describe critical opalescence[4].

1. The linear, but non-local response to a small external field.

2. "Soliton" or domain wall solutions, in which the order parameter changes sign, passing through the maximum in the free energy at $\psi = 0$. (Such domain walls are particular to Ising order).

To obtain the equation governing non-uniform solutions, we write

$$\delta F_{GL} = \int d^d x\, \delta\psi(x) \left[-s\nabla^2\psi(x) + \frac{\partial f_L[\psi]}{\partial \psi(x)} \right]. \tag{12.15}$$

Since the Ginzburg Landau free energy must be stationary with respect to small variations in the field:

$$\frac{\delta F_{GL}}{\delta\psi(x)} = -s\nabla^2\psi + \frac{\partial f_L[\psi]}{\partial\psi} = 0 \tag{12.16}$$

or more explicitly

$$\boxed{\left[(-s\nabla^2 + r) + u\psi^2\right]\psi(x) - h(x) = 0} \tag{12.17}$$

Susceptibility and linear response

The simplest application of GL theory, is to calculate the linear response to a non-uniform applied field. For $T > T_c$, for a small linear response we can neglect the cubic term so that $(-c\nabla^2 + r)\psi(x) = h(x)$. If we Fourier transform this equation, we obtain

$$(sq^2 + r)\psi_{\mathbf{q}} = h_{\mathbf{q}} \tag{12.18}$$

or $\psi_q = \chi_{\mathbf{q}} h_{\mathbf{q}}$, where

$$\chi_{\mathbf{q}} = \frac{1}{sq^2 + r} = \frac{1}{s(q^2 + \xi^{-2})} \tag{12.19}$$

is the momentum-dependent susceptibility and $\xi = \sqrt{s/r}$ is the correlation length defined in (12.14). Notice that $\chi_{\mathbf{q}=0} = 1/[a(T - T_c)] = r^{-1}$ is the uniform susceptibility obtained in (12.9) earlier. For large $q >> \xi^{-1}$, $\chi(q) \sim 1/q^2$ becomes strongly momentum dependent: in otherwords, the response to an applied field is non-local up to a the correlation length.

Example 12.2:

(a) Show that in $d = 3$ dimensions, for $T > T_c$, the response of the order parameter field to an applied field is non-local, and given by

$$\psi(x) = \int d^3x' \chi(x - x')h(x')$$
$$\chi(x - x') = \frac{\chi}{4\pi\xi^2}\frac{e^{-|x-x'|/\xi}}{|x - x'|} \tag{12.20}$$

(b) Show that provided $h(x)$ is slowly varying on scales of order ξ, the linear response can be approximated by

$$\psi(x) = \chi h(x)$$

Solution:

(a) If we carry out the inverse Fourier transform of the response $\psi(q) = \chi(q)h(q)$, we obtain

$$\psi(x) = \int_{x'} \chi(x - x')h(x')$$

In example (4.6) we showed that under a Fourier transform

$$\frac{e^{-\lambda|x|}}{|x|} \overset{\text{FT}}{\to} \frac{4\pi}{q^2 + \lambda^2}$$

so the (inverse) Fourier transform of the non-local susceptibility is

$$\chi(q) = \frac{c^{-1}}{q^2 + \xi^{-2}} \overset{\text{FT}^{-1}}{\to} \frac{1}{4\pi s}\frac{e^{-|x|/\xi}}{|x|} = \frac{\chi}{4\pi\xi^2}\frac{e^{-|x|/\xi}}{|x|}$$

(b) At small q, we may replace $\chi(q) \approx \chi$, so that for slowly varying h in real space we can replace $\chi(x - x') \to \chi\delta^{(d)}(x - x')$. So that provided h is slowly varying over lengths longer than the correlation length, $\psi(x) = \chi h(x)$.

Domain Walls

Once $T < T_c$, it is energetically costly for the order parameter to deviate seriously from the equilibrium values ψ_0. Major deviations from these "stable vacua" can however take place at "domain walls" or "solitons", which are narrow walls of space which separate the two stable "vacua" of opposite sign, where $\psi = \pm\psi_0$. To change sign, and Ising order parameter must pass through zero at the center of the domain wall, passing over the "hump" in the free energy.

We now solve for the soliton in one dimension, where the Ginzburg Landau equation becomes

$$c\psi'' = \frac{df_L[\psi]}{d\psi}. \tag{12.21}$$

This formula has an intriguing interpretation as Newton's law of motion for a particle of mass c moving in an inverted potential $V[\psi] = -f_L[\psi]$. This observation permits an analogy between a

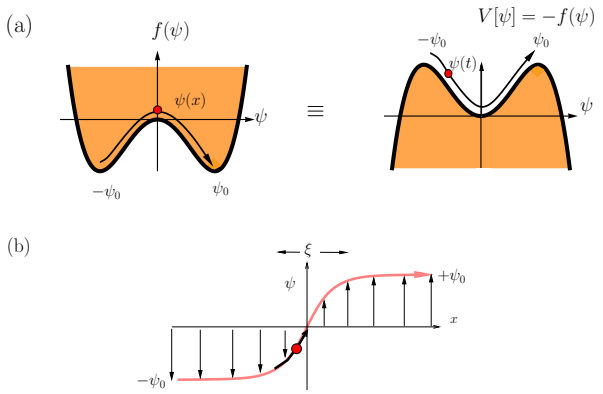

Figure 12.6: Soliton solution of Ginzburg Landau equations. (a) The evolution of ψ in one dimension is equivalent to a particle at position ψ, moving in an inverted potential $V[\psi] = -f_L[\psi]$. A soliton is equivalent to a "bounce" between maxima at $\psi = \pm\psi_0$ of $V[\psi]$. (b) The "path" that the particle traces out in time "t" $\equiv x$ defines the spatial dependence of the order parameter $\psi[x]$.

soliton and and motion in one dimension which enables us to to quickly develop a solution for the soliton. In this analogy, ψ plays the role of displacement while x plays the role of time. It follows that $\frac{s}{2}(\psi')^2$ is an effective "kinetic energy" [3] and the effective "energy"

$$\mathcal{E} = \frac{s}{2}(\psi')^2 - f_L[\psi]$$

is conserved and independent of x. With our simple analogy, we can map a soliton onto the problem of a particle rolling off one maxima of the inverted potential $V[\psi] = -f_L[\psi]$, "bouncing" through $\psi = 0$ out to the other maxima (Fig12.6). Fixing the conserved initial energy to be $\mathcal{E} = -f_L[\psi_0]$, we deduce the "velocity"

$$\psi' = \frac{d\psi}{dx} = \sqrt{\frac{2}{s}(\mathcal{E} + f_L[\psi])} = \frac{\psi_0}{\sqrt{2}\xi}\left(1 - \frac{\psi^2}{\psi_0^2}\right),$$

To make the last step we have replaced $\psi_0^2 = \frac{|r|}{u}$ and $\xi = \sqrt{\frac{s}{|r|}}$. Solving for $dx = (\sqrt{2}\xi/\psi_0)[1 - (\tilde{\psi}/\psi_0)^2]^{-\frac{1}{2}}d\psi$ and integrating both sides yields

$$x - x_0 = \frac{\sqrt{2}\xi}{\psi_0}\int_0^{\psi}\frac{d\tilde{\psi}}{1-(\tilde{\psi}/\psi_0)^2} = \sqrt{2}\xi\tanh^{-1}(\psi/\psi_0),$$

where $x = x_0$ is the point where the order parameter passes through zero, so that

$$\psi(x) = \psi_0\ \tanh(\frac{x - x_0}{\sqrt{2}\xi}). \qquad \textbf{"soliton"}$$

This describes a "soliton" solution to the Ginzburg Landau located at $x = x_0$.

[3] This can be derived by multiplying (12.21) by the integrating factor ψ' then

$$c(\psi'\psi'') - \psi'\frac{df_L[\psi]}{d\psi} = \frac{d}{dx}\left[\frac{s}{2}(\psi')^2 - f_L[\psi]\right] = 0.$$

Example 12.3: Show that the Ginzburg Landau free energy of a Domain wall can be written

$$\Delta F = A\frac{u}{4}\int dx[\psi_0^4 - \psi^4(x)]$$

where $A = L^{d-1}$ is the area of the domain wall. Using this result, show that surface tension $\sigma = \Delta F/A$ is given by

$$\sigma = \frac{\sqrt{8}}{3}\xi u\psi_0^4.$$

Solution: First, let us integrate by parts to write the total energy of the domain in the form

$$F = A\int dx\left[-\frac{s}{2}\psi\psi'' + f_L[\psi]\right] \tag{12.22}$$

where for $r < 0$, $f_L[\psi] = -\frac{|r|}{2}\psi^4 + \frac{u}{4}\psi^4$ Using the GL equation (12.21)

$$s\psi'' = \frac{df_L}{d\psi} = -|r|\psi + u\psi^3.$$

Subsituting into (12.22), we obtain

$$\begin{aligned} F &= -A\int dx\left[-\frac{1}{2}\psi\left(-|r|\psi + u\psi^3\right) - \frac{|r|}{2}\psi^2 + \frac{u}{4}\psi^4\right] \\ &= -uA\int dx\psi^4(x) \end{aligned} \tag{12.23}$$

Subtracting off the energy of the uniform configuration, we then obtain

$$\Delta F = A\frac{u}{4}\int dx(\psi_0^4 - \psi^4(x))$$

To calculate the surface tension, substitute $\psi(x) = \psi_0\tanh[x/(\sqrt{2}\xi)]$, which gives

$$\sigma = \frac{\Delta F}{A} = \frac{u}{4}\psi_0^4\int_{-\infty}^{\infty}dx(1 - \tanh[x/(\sqrt{2}\xi)^4)$$

$$= \frac{\xi u}{\sqrt{8}}\psi_0^4 \overbrace{\int_{-\infty}^{\infty} du(1-\tanh[u]^4)}^{8/3} = \frac{\sqrt{8}}{3}\xi u\psi_0^4. \qquad (12.24)$$

12.4 Landau Ginzburg II: Complex order and Superflow

12.4.1 "A macroscopic wavefunction"

We now turn to discuss the Ginzburg Landau theory of complex, or two component order parameters. Here, we shall focus on the use of Ginzburg Landau theory to understand superfluids and superconductors. At the heart of our discussion, is the emergence of a kind of "macroscopic wavefunction" in which the microscopic field operators of the quantum fluid $\hat{\psi}(x)$ acquire an expectation value

$$\langle\hat{\psi}(x)\rangle \equiv \psi(x) = |\psi(x)|e^{i\phi(x)} \qquad \text{"Macroscopic wavefunction"}$$

complete with phase. The magnitude of this order parameter determines the density of particles in the superfluid

$$|\psi(x)|^2 = n_s(x)$$

while the twist, or gradient of the phase determines the superfluid velocity.

$$\mathbf{v}_s(x) = \frac{\hbar}{m}\nabla\phi(x).$$

The idea that the wavefunction can acquire a kind of Newtonian reality in a superfluid or superconductor goes deeply against our training in quantum physics: at first sight, it appears to defy the Copenhagen interpretation of quantum mechanics, in which $\psi(x)$ is an unobservable variable. The bold idea suggested by Ginzburg Landau is that $\psi(x)$ is a macroscopic manifestation of quintillions of particles - bosons - all condensed into precisely the same quantum state. Even the great figures of the field - Landau himself - found this hard to absort, and debate continues today. Yet on his issue, history and discovery appear to consistently have sided with the bold, if perhaps naive, interpretation of the superconducting and superfluid order parameter as a essentially real, observable property of quantum fluids [4]. It is the classic example of an *"emergent phenomenon"* - one of the many collective properties of matter that we are still discovering today which is a not *a priori* self-evident from the microscopic physics.

[4] On more than one occasion, senior physicists advised their students and younger colleagues against such a brash interpretation. One such story took place in Moscow in 1953. Shortly after Ginzburg Landau theory was introduced, a young student of Landau, Alexei Abrikosov showed that a naive classical interpretation of the order parameter field led naturally to the predication of quantized vortices and superconducting vortex lattices. Landau himself could not bring himself to make this leap and persuaded his student to shelve the theory. It was only after Feynman published a theory of vortices in superfluid helium, that Landau accepted the idea, clearing the way for Abrikosov to finally publish his paper. [6]

Vitalii Ginzburg and Lev Landau introduced their theory in 1950, as a phenomenological theory of superconductivity, in which $\psi(x)$ played the role of a macroscopic wavefunction whose microscopic origin was, at the time, unknown. We shall begin by illustrating the application of with an application of this method to superfluids. For a superfluid, the GL free energy density is

$$f_{GL}[\psi,\nabla\psi] = \frac{\hbar^2}{2m}|\nabla\psi|^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4, \qquad (12.25)$$

GL free energy: superfluid

Before continuing, let us make a few heuristic remarks about the GL free energy:

- The the GL free energy is to be interpreted as the energy density of a condensate of bosons in which the field operator behaves as a complex order parameter. This leads us to identify the coefficient of the gradient term

$$s|\nabla\psi|^2 \equiv \frac{\hbar^2}{2m}\left\langle\nabla\hat{\psi}^\dagger\nabla\hat{\psi}\right\rangle \qquad (12.26)$$

  as the kinetic energy, so that $s = \frac{\hbar^2}{2m}$.

- As in the case of Ising order, the correlation length, or "Ginzburg Landau coherence length" governing the characteristic range of amplitude fluctuations of the order parameter is given by

$$\xi = \sqrt{\frac{s}{|r|}} = \sqrt{\frac{\hbar^2}{2M|r|}} = \xi_0\left(1-\frac{T}{T_c}\right)^{-1/2} \qquad (12.27)$$

  where $\xi_0 = \xi(T=0) = \sqrt{\frac{\hbar^2}{2maT_c}}$ is the coherence length. Beyond this length-scale, only phase fluctuations survive.

- If we freeze out fluctuations in amplitude, writing $\psi(x) = \sqrt{n_s}e^{i\phi(x)}$, then $\nabla\psi = i\nabla\phi\,\psi$ and $|\nabla\psi|^2 = n_s(\nabla\phi)^2$, the residual dependence of the kinetic energy on the twist in the phase is

$$\frac{\hbar^2 n_s}{2m}(\nabla\phi)^2 = \frac{mn_s}{2}\overbrace{\left(\frac{\hbar}{m}\nabla\phi\right)^2}^{\mathbf{v}_s^2}.$$

  Since mn_s is the mass density, we see that a twist of the phase results in an increase in the kinetic energy that we may associate with a "superfluid" velocity

$$\mathbf{v_s} = \frac{\hbar}{m}\nabla\phi.$$

12.4.2 Off-diagonal long range order and coherent states

What then, is the meaning of the complex order parameter ψ? It is tempting to associate it with the expectation value of the field operator

$$\langle\hat{\psi}(x,t)\rangle = \psi(x,t)$$

Yet, paradoxically, a field operator, links states with different particle numbers, so such an expectation value can never develop in a state in a state with a definite number of particles. One way to avoid this problem, proposed by Penrose and Onsager, is to define the order parameter in terms of correlation functions[7, 8]. The authors noted that even in a state with a definite particle number, broken symmetry manifests itself as a long-distance factorization [9] of the correlation function $\langle\psi^\dagger(x)\psi(x)\rangle$:

$$\langle\psi^\dagger(x')\psi(x)\rangle \xrightarrow{|x'-x|\gg\xi} \psi^*(x')\,\psi(x) + \text{small terms} \qquad (12.28)$$

Off-diagonal long range order.

in terms of the order parameter. This property is called "off-diagonal long range order" [10](ODLRO).

However, a more modern view is that in macroscopic systems, we don't need to restrict our attention to to states of definite particle number, and indeed, once we bring a system into contact with a bath of particles, quantum states of indefinite particle number do arise. This issue also arises in a ferromagnet where, the analog of particle number is the conserved magnetization S_z along the z-axis. A ferromagnet of N spins polarized in the z direction has wavefunction

$$|Z\rangle = \prod_{\substack{\otimes\\ i=1,N}} |\uparrow\rangle_i$$

However, if we cool the magnet in a field aligned along the x-axis, coupled via the Hamiltonian $H = -2BS_x = -B(S^+ + S^-)$, then once we remove the field at low temperatures, the magnet remains polarized in the x direction:

$$|X\rangle = \prod_{\substack{\otimes\\ i=1,N}} |\rightarrow\rangle_i = \prod_{\substack{\otimes\\ i=1,N}} \left(\frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}\right)_i .$$

Thus the coherent exchange of spin with the environment leads to a state that contains an admixture of states of different S_z. In a similar way, we may consider cooling a quantum fluid in a field that couples to the superfluid order parameter. Such a field is created by a "proximity effect" of the exchange of particles with a pre-cooled superfluid in close vicinity, giving rise to a field term in the Hamiltonian such as

$$H' = -\Delta \int d^dx[\psi^\dagger(x) + \psi(x)]$$

When we cool below the superfluid transition temperature T_c in the presence of this pairing field, removing the proximity field at low temperatures, then like a magnet, the resulting state acquires

an order parameter forming a stable state of indefinite particle number. [5] To describe such states requires the many body equivalent of wave-packets: a type of state called a "coherent state".

Coherent states are eigenstates of the field operator

$$\hat{\psi}(x)|\psi\rangle = \psi(x)|\psi\rangle. \qquad (12.29)$$

These states form an invaluable basis for describing superfluid states of matter. A coherent state can be simply written as

$$|\psi\rangle \sim e^{\sqrt{N_s}b^\dagger}|0\rangle \qquad \textbf{coherent state}. \qquad (12.30)$$

where

$$b^\dagger = \frac{1}{\sqrt{N_s}}\int d^dx\,\psi(x)\hat{\psi}^\dagger(x),$$

coherently adds a boson to a condensate with with wavefunction $\psi(x)$. Here, $N_s = \int d^dx|\psi(x)|^2$ is the *average* number of bosons in the superfluid and the normalization is chosen so that $[b, b^\dagger] = 1$. (See example 13.4 and exercise 13.6.)

Similarly, the conjugate state $\langle\psi| = \langle 0|e^{\sqrt{N_s}\hat{b}}$ diagonalizes the creation operator:

$$\langle\psi|\hat{\psi}^\dagger(x) = \psi^*(x)\langle\psi|. \qquad (12.31)$$

However, it not possible to simultaneously diagonalize both creation and annihilation operators because they don't commute. Thus $|\psi\rangle$ *only* diagonalizes the destruction operator and $\langle\psi^*|$ only diagonalizes the creation operator.

Coherent states are really the many body analog of "wave-packets", with the roles of momentum and position replaced by N and ϕ respectively. Just as $\hat{p}$ generates spatial translations ,$e^{-iPa/\hbar}|x\rangle = |x + a\rangle$, $\hat{N}$ translates the phase (see exercise 1), so that $e^{i\alpha\hat{N}}|\phi\rangle = |\phi + \alpha\rangle$. (Notice the difference in the sign in the exponent). For an infinitesimal phase translation $\langle\phi + \delta\phi| = \langle\phi|(1 - i\delta\phi\hat{N})$, so $i\frac{d}{d\phi}\langle\phi| = \langle\phi|\hat{N}$, implying

$$\hat{N} = i\frac{d}{d\phi}.$$

This is the many body analog of the identity $\hat{p} \equiv -i\hbar\frac{d}{dx}$. Just as periodic boundary conditions in space give rise to discrete quantized values of momentum, the periodic nature of phase, gives rise to a quantized particle number. It follows that

$$[\hat{N}, \hat{\phi}] = i$$

implying phase and particle number are conjugate variables which obey an uncertainty relation [6]

$$\Delta\phi\Delta N \gtrsim 1$$

[5] One might well object to this line of reasoning - for clearly, creating a state with a definite phase requires we have another pre-cooled superfluid prepared in a state of definite phase. But what happens if we have none to start with? It turns out that what we really can do, is to control the relative phase of two superfluids. By field-cooling, and it is the relative phase that we can actually measure.

[6] The strict relation is $\Delta\phi\Delta N \geq \frac{1}{2}|[\hat{\phi}, \hat{N}]| = \frac{1}{2}$. As in the case of wavepackets, in heuristic discussion, we drop the factor of one half.

A coherent state trades in a small fractional uncertainty in particle number to gain a high degree of precision in its phase. For small quantum systems where the uncertainty in particle number is small, phase becomes ill-defined. If we write the uncertainty principle in terms of the relative error $\Delta\epsilon = \Delta N/N$, then $\Delta\phi\Delta\epsilon \gtrsim 1/N$ we see that once $N \sim 10^{23}$, the fractional uncertainty in particle number and the phase can be known to an accuracy of order 10^{-11}. In the thermodynamic limit this means we can localize and measuring both the phase and the particle density with Newtonian precision.

Example 12.4: The coherent state (12.30) is not normalized. Show that the properly normalized coherent state

$$\begin{aligned} |\psi\rangle &= e^{-N_s/2} e^{\sqrt{N_s} b^\dagger}|0\rangle, \\ b^\dagger &= \frac{1}{\sqrt{N_s}}\int_x \psi(x)\hat\psi^\dagger(x) \end{aligned} \tag{12.32}$$

is an eigenstate of the annihilation operator $\hat\psi(x)$ with eigenvalue $\psi(x)$, where $N_s = \int d^d x|\psi(x)|^2$.

Solution:

1. First, since $[\hat\psi(x), \hat\psi^\dagger(x')] = \delta^{(d)}(x-x')$, we note that

$$[b, b^\dagger] = \frac{1}{N_s}\int_{x,x'} \psi(x)\psi^*(x')\overbrace{[\hat\psi(x), \hat\psi^\dagger(x')]}^{\delta^{(d)}(x-x')} = \frac{1}{N_s}\int_x |\psi(x)|^2 = 1,$$

   so that b and $b^\dagger$ are canonical bosons.

2. To obtain the normalization of a coherent state, let us expand the exponential in $|z\rangle = e^{z\hat b^\dagger}|0\rangle$ in terms of eigenstates of the boson number operator $\hat n = b^\dagger b$, $|n\rangle$, as follows:

$$|z\rangle = \sum_{n=0}^\infty \frac{(zb^\dagger)^n}{n!}|0\rangle = \sum_{n=0}^\infty \frac{z^n}{\sqrt{n!}}\overbrace{\frac{(b^\dagger)^n}{\sqrt{n!}}|0\rangle}^{|n\rangle} = \sum_{n=0}^\infty \frac{z^n}{\sqrt{n!}}|n\rangle$$

   Since $\langle n'|n\rangle = \delta_{n,n'}$, taking the norm, we obtain

$$\langle z|z\rangle = \sum_n \frac{|z|^n}{n!} = e^{|z|^2}$$

   Placing $z = \sqrt{N_s}$, it follows that the normalized coherent state is $|\psi\rangle = e^{-N_s/2} e^{\sqrt{N_s} b^\dagger}|0\rangle$.

3. Since $\hat\psi(x)|0\rangle = 0$, the action of the field operator on the coherent state is

$$\hat\psi(x)|\psi\rangle = e^{-N_s/2}[\hat\psi(x), e^{\sqrt{N_s} b^\dagger}]|0\rangle \tag{12.33}$$

   To simplify notation, let us denote $\alpha^\dagger = \sqrt{N_s} b^\dagger$. The commutator

$$[\hat\psi(x), \alpha^\dagger] = \int_{x'} \psi(x')\overbrace{[\hat\psi(x), \hat\psi^\dagger(x')]}^{\delta^{(d)}(x-x')} = \psi(x)$$

which in turn implies that $[\hat\psi(x), (\alpha^\dagger)^r] = r\psi(x)(\alpha^\dagger)^{r-1}$. Now expanding

$$e^{\alpha^\dagger} = \sum_r \frac{1}{r!}(\alpha^\dagger)^r$$

we find that

$$[\hat\psi(x), e^{\hat\alpha^\dagger}] = \sum_{r=0}^\infty \frac{1}{r!}[\hat\psi(x), (\hat\alpha^\dagger)^r] = \psi(x)\sum_{r=1}^\infty \frac{(\hat\alpha^\dagger)^{r-1}}{(r-1)!} = \psi(x)e^{\hat\alpha^\dagger}$$

so that finally,

$$\hat\psi(x)|\psi\rangle = e^{-N_s/2}[\hat\psi(x), e^{\sqrt{N_s} b^\dagger}]|0\rangle = \psi(x)e^{-N_s/2}e^{\sqrt{N_s} b^\dagger}|0\rangle = \psi(x)|\psi\rangle. \tag{12.34}$$

Ginzburg Landau energy for a coherent state

We shall now link the one-particle wavefunction of the condensate to the order parameter of Ginzburg Landau theory. While coherent states are not perfect energy eigenstates, at high density they provide an increasingly accurate description of the ground-state wavefunction of a condensate. To take the expectation value of normal ordered operators between coherent states, one simply replaces the fields by the order parameter, so that if

$$\hat{\mathcal{H}} = \frac{\hbar^2}{2m}\nabla\hat\psi^\dagger(x)\nabla\hat\psi(x) + (U(x)-\mu)\hat\psi^\dagger(x)\hat\psi(x) + \frac{u}{2}:(\hat\psi^\dagger(x)\hat\psi(x))^2: \tag{12.35}$$

is the energy density of the microscopic fields, where $U(x)$ is the one-particle potential, then the energy density of the condensate is

$$\langle\psi|\mathcal{H}[\hat\psi^\dagger, \hat\psi]|\psi\rangle = \mathcal{H}[\psi^*, \psi] = \frac{\hbar^2}{2m}|\nabla\psi(x)|^2 + (U(x)-\mu)|\psi(x)|^2 + \frac{u}{2}|\psi(x)|^4.$$

which we recognize as a Ginzburg Landau energy density with

$$s = \frac{\hbar^2}{2m}, \qquad r(x) = U(x) - \mu.$$

At a finite temperature, this analysis needs modification. For instance, μ will acquire a temperature dependence that permits $r(T)$ to vanish at T_c, while the relevant functional becomes free energy $F = E - TS$. Finally, note that at a finite temperature, $n_s(T)$ only defines the superfluid component of the total particle density n, which contains both a normal and a superfluid component $n = n_s(T) + n_n(T)$.

12.4.3 Phase rigidity and superflow

In GL theory the energy is sensitive to a "twist" of the phase. If we substitute $\psi = |\psi|e^{i\phi}$ into the GL free energy, the gradient term becomes $\nabla\psi = (\nabla|\psi| + i\nabla\phi|\psi|)e^{i\phi}$, so that

$$f_{GL} = \overbrace{\frac{\hbar^2}{2m}|\psi|^2(\nabla\phi)^2}^{\textbf{KE: phase rigidity}} + \overbrace{\left[\frac{\hbar^2}{2m}(\nabla|\psi|)^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4\right]}^{\text{amplitude fluctuations}} \tag{12.36}$$

The second term resembles the Ginzburg Landau functional for an Ising order parameter, and describes the energy cost of variations in the magnitude of the order parameter. The first term term is new. This term describes the **"phase rigidity"**. As we learnt in the previous section, amplitude fluctuations of the order parameter are confined to scales shorter than the correlation length ξ. On longer length-scales the physics is entirely controlled by the phase degrees of freedom, so that

$$f_{GL} = \frac{\rho_\phi}{2}(\nabla\phi)^2 + \text{constant} \tag{12.37}$$

The quantity $\rho_\phi = \frac{\hbar^2}{m}n_s$ is often called the "superfluid phase stiffness".

From a microscopic point of view, the phase rigidity term is simply the kinetic energy of particles in the condensate, but from a macroscopic view, it is an elastic energy associated with the twisted phase. The only way to reconcile these two viewpoints, is if a twist of the condensate wavefunction results in a coherent flow of particles.

To see this explicitly, let us calculate the current in a coherent state. Microscopically, the current operator is

$$\vec{J} = -i\frac{\hbar}{2m}\left(\hat{\psi}^\dagger\vec{\nabla}\hat{\psi} - \vec{\nabla}\hat{\psi}^\dagger\hat{\psi}\right)$$

so in a coherent state,

$$\langle\psi|\vec{J}|\psi\rangle = -i\frac{\hbar}{2m}\left(\psi^*\vec{\nabla}\psi - \vec{\nabla}\psi^*\psi\right) \tag{12.38}$$

If we substitute $\psi(x) = \sqrt{n_s(x)}e^{i\phi(x)}$ into this expression, we find that

$$\mathbf{J}_s = n_s\frac{\hbar}{m}\nabla\phi \tag{12.39}$$

so that constant twist of the phase generates a flow of matter. Writing $\mathbf{J}_s = n_s\mathbf{v}_s$, we can identify

$$\mathbf{v}_s = \frac{\hbar}{m}\nabla\phi.$$

as the "superfluid velocity" generated by the twisted phase of the condensate. Conventional particle flow is acheived by the addition of excitations above the ground-state, but superflow occurs through a deformation of the ground-state phase and every single particle moves in perfect synchrony.

Example 12.5:

(a) Show that in a condensate, the quantum equations of motion for the phase and particle number can be replaced by Hamiltonian dynamics[9]:

$$\begin{aligned}\hbar\frac{dN}{dt} &= i[N,H] = \frac{\partial H}{\partial\phi}\\ \hbar\frac{d\phi}{dt} &= i[\phi,H] = -\frac{\partial H}{\partial N}\end{aligned} \tag{12.40}$$

which are the analog of $\dot{q} = \frac{\partial H}{\partial p}$ and $\dot{p} = -\frac{\partial H}{\partial q}$.

(b) Use the second of the above equations to show that in a superfluid at chemical potential μ, the equilibrium order parameter will precess with time, according to

$$\psi(x,t) = \psi_(x,0)e^{-i\mu t/\hbar}$$

(c) If two superfluids with the same superfluid density, but at different chemical potentials μ_1 and μ_2 are connected by a tube of length L show that the superfluid velocity from $1 \to 2$ will "accelerate" according to the equation

$$\frac{dv_s}{dt} = -\frac{\hbar}{m}\frac{\mu_2 - \mu_1}{L}$$

Solution:

(a) Since $[\phi, \hat{N}] = i$, there are two alternative representations of the operators:

$$\hat{N} = -i\frac{d}{d\phi}, \qquad \hat{\phi} = \phi \tag{12.41}$$

or, in the case that N is large enough to be considered a continuous variable,

$$\hat{\phi} = i\frac{d}{dN}, \qquad \hat{N} = N \tag{12.42}$$

Using (12.41), the Heisenberg equation of motion for $N(t)$ is given by

$$\frac{dN}{dt} = \frac{i}{\hbar}[N,H] = \frac{i}{\hbar}[-i\frac{d}{d\phi}, H(N,\phi)] = \frac{1}{\hbar}\frac{\partial H}{\partial\phi} \tag{12.43}$$

while using (12.42), the Heisenberg equation of motion for $\phi(t)$ is given by

$$\frac{d\phi}{dt} = \frac{i}{\hbar}[\phi,H] = \frac{i}{\hbar}[i\frac{d}{dN}, H] = -\frac{1}{\hbar}\frac{\partial H}{\partial N}, \tag{12.44}$$

(b) In a bulk superfluid, $\frac{\partial H}{\partial N} = \mu$, so using (12.44), $\dot{\phi} = \mu/\hbar$, and hence $\phi(t) = -\frac{\mu t}{\hbar} + \phi_0$, or

$$\psi(x,t) = \psi(x,0)e^{-i\mu t/\hbar}$$

(c) Assuming a constant gradient of phase along the tube connecting the two superfluids, the superfluid velocity is given by

$$v_s = \frac{\hbar}{m}\nabla\phi(t) = \frac{\hbar}{m}(\phi_2(t) - \phi_1(t))/L$$

But $\phi(2) - \phi(1) = -(\mu_2 - \mu_1)t + \text{cons}$, hence

$$\frac{dv_s}{dt} = -\frac{\hbar}{m}\frac{\mu_2 - \mu_1}{L}$$

Vortices and topological stability of superflow

Superflow is stable because of the underlying topology of a twisted order parameter. If we wrap the system around on itself then the the single-valued nature of the order parameter implies that the change in phase around the sample must be an integer multiple of 2π:

$$\Delta\phi = \oint d\mathbf{x}\cdot\nabla\phi = 2\pi \times n_\phi$$

corresponding to n_ϕ twists of the order parameter. But since $v_s = \frac{\hbar}{m}\nabla\phi$, this implies that line-integral, or "circulation" of the superflow around the sample is quantized

$$\omega = \oint d\mathbf{x}\cdot\mathbf{v}_s = \frac{h}{m}\times n_\phi \qquad \textit{quantization of circulation}$$

(note h without a slash). Assuming translational symmetry, this implies

$$v_s = \frac{h}{mL}n_\phi \qquad \textit{quantization of velocity,}$$

a phenomenon first predicted by Onsager and Feynman[11, 12]. The number of twists of the order parameter n_ϕ is a "topological invariant" of the superfluid condensate, since it can not be changed by any continuous deformation of the phase. The only way to decay the superflow is to create high energy domain walls: a process that is exponentially suppressed in the thermodyanmic limit. Thus the topological stability of a twisted order parametery sustains a persistent superflow.

Another topologically stable configuration of a superfluid is a "vortex". A vortex is a singular line in the superfluid around which the phase of the order parameter precesses by an integer multiple of 2π. If we take a circular path of radius r around the vortex then the quantization of circulation implies

$$\omega = n_\phi\left(\frac{h}{m}\right) = \oint d\mathbf{x}\cdot\mathbf{v}_s(x) = 2\pi r v_s$$

or

$$v_s = n_\phi \times \left(\frac{\hbar}{m}\right)\frac{1}{r}, \qquad (r \gtrsim \xi)$$

This formula, where the superfluid velocity appears to diverge at short distances, is no longer reliable for $r \lesssim \xi$, where amplitude variations in the order parameter become important.

Let us now calculate the energy of a vortex. Suppose the vortex is centered in the middle of a large cylinder of radius R, then the energy per unit length is

$$\frac{F}{L} = \frac{\rho_\phi}{2}\int d^2x(\nabla\phi)^2 = \frac{\rho_\phi}{2}\int_\xi^R 2\pi r dr\left(\frac{2\pi n_\phi}{2\pi r}\right)^2 = \pi\rho_\phi \ln\left(\frac{R}{\xi}\right)\times n_\phi^2.$$

In this way, we see that the energy of n_ϕ isolated vortices with unit circulation, is n_ϕ times smaller than one vortex with n_ϕ-fold circulation. For this reason, vortices occur with single quanta of circulation, and their interaction is repulsive.

12.5 Landau Ginzburg III: Charged fields

12.5.1 Gauge Invariance

In a neutral superfluid the emergence of a macrosopic wavefunction with a phase leads superfluidity. When the corresponding fluid is charged, the superflow carries charge, forming a superconductor. One of the key properties of superconductors, is their ability to actively exclude magnetic fields from their interior, a phenomenon called the "Meissner effect". Ginzburg Landau theory provides a beautiful account of this effect.

The introduction of charge into a field theory brings with it the notion of gauge invariance. From one-body Schrödinger equation,

$$i\hbar\frac{\partial\psi}{\partial t} = \left[-\frac{\hbar^2}{2m}\left(\nabla - i\frac{e}{\hbar}\mathbf{A}\right)^2 + e\varphi(x)\right]\psi$$

where φ is the scalar electric potential, we learn that we can change the phase of a particle wavefunction by an arbitrary amount at each point in space and time, $\psi(x,t) \to e^{i\alpha(t)}\psi(x,t)$ without without altering the equation of motion, so long as the change is compensated by a corresponding gauge transformation of the electromagnetic field:

$$\mathbf{A} \to \mathbf{A} + \frac{\hbar}{e}\nabla\alpha, \qquad \varphi \to \varphi - \frac{\hbar}{e}\frac{\partial\alpha}{\partial t}. \tag{12.45}$$

This intimate link between changes in the phase of the wavefunction and gauge transformations of the electromagnetic field threads through all of many body physics and field theory. Once we second-quantize quantum mechanics, the same rules of gauge invariance apply to the fields that create charged particles, and when these fields, or combinations of them condense, the corresponding charged order parameter also obeys the rules of gauge invariance, with the proviso that the charge e^* is the charge of the condensate field. These kinds of arguments imply that in the Ginzburg Landau theory of a charged quantum fluid, normal derivatives of the field are replaced by gauge invariant derivatives

$$\nabla \to \mathbf{D} = \nabla - \frac{ie^*}{\hbar}\mathbf{A}$$

where e^* is the charge of the condensing field. Thus the simple replacement

$$f_{GL}[\psi, \nabla\psi] \to f_{GL}[\psi, \mathbf{D}\psi]$$

incorporates the coupling of the superfluid to the electromagnetic field. To this, we must add the energy density of the magnetic field $\mathbf{B}^2/(2\mu_0)$, to obtain

$$F[\psi, \mathbf{A}] = \int d^dx \Big[\overbrace{\frac{\hbar^2}{2M}\Big|(\nabla - \frac{ie^*}{\hbar}\mathbf{A})\psi\Big|^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4}^{f_\psi} + \underbrace{\frac{(\nabla\times\mathbf{A})^2}{2\mu_0}}_{f_{EM}} \Big] \tag{12.46}$$

GL Free energy: charged superfluid.

where M is mass of the condensed field and $\nabla \times \mathbf{A} = \mathbf{B}$ is the magnetic field.

Note that:

- So long as we are considering superconductors, where the condensing boson is a Cooper pair of electrons, $e^* = 2e$. Although there are cases of charged bosonic superfluids, such as a fluid of deuterium nucleii, in which $e^* = e$, for the rest of this book, we shall adopt

  $$e^* \equiv 2e \tag{12.47}$$

  as an equivalence.

- Under the gauge transformation

  $$\psi(x) \to \psi(x)e^{i\alpha(x)}, \qquad \mathbf{A} \to \mathbf{A} + \frac{\hbar}{e^*}\nabla\alpha$$

  $\mathbf{D}\psi \to e^{i\alpha(x)}\mathbf{D}\psi$, so that $|\mathbf{D}\psi|^2$ is unchanged and the GL free energy is gauge invariant.

- $F[\psi, A]$ really contains *two* intertwined Ginzburg Landau theories for ψ and A respectively, with two corresponding length scales: the coherence length $\xi = \sqrt{\frac{\hbar^2}{2M|r|}}$ governing amplitude fluctuations of ψ and and the "London penetration depth" λ_L, which sets the distance a magnetic field penetrates into the superconductor. In a uniform condensate $\psi = \sqrt{n_s}$, the free energy dependence on the vector potential is given by

  $$f[\mathbf{A}] \sim c_A\frac{(\nabla\times\mathbf{A})^2}{2} + \frac{r_A}{2}\mathbf{A}^2, \tag{12.48}$$

  where $c_A = \frac{1}{\mu_0}$ and $r_\mathbf{A} = \frac{e^{*2}n_s}{M}$. This is a Ginzburg Landau functional for the vector potential with a characteristic **London penetration depth**

  $$\lambda_L = \sqrt{\frac{c_\mathbf{A}}{r_\mathbf{A}}} = \sqrt{\frac{M}{n_s e^{*2}\mu_0}}, \tag{12.49}$$

12.5.2 Ginzburg Landau Equations

To obtain the equations of motion we need to take variations of the free with respect to the vector potential and the order parameter ψ. Variations in the vector potential recover Ampères equation, while variations in the order parameter lead to a generalization of the non-linear Schrodinger equation obtained previously for non-uniform Ising fields. Each of these equations is of great importance - non-uniform solutions determine the physics of the domain walls between "normal" and "superconducting" regions of a type II superconductor, while the Ginzburg Landau formulation of Ampère's equation provides an understanding of the Meissner effect.

If we vary the vector potential, then $\delta F = \delta F_\psi + \delta F_{EM}$, where

$$\delta F_\psi = -\int_x \delta\mathbf{A}(x)\cdot\overbrace{\Big[-\frac{i\hbar}{2M}\big(\psi^*\vec{\nabla}\psi - \vec{\nabla}\psi\,\psi\big) - \frac{e^{*2}}{M}|\psi|^2\Big]}^{\mathbf{J}(x)}$$

is the variation in the condensate energy and [7]

$$\delta F_{EM} = \frac{1}{\mu_0}\int \nabla\times\delta\mathbf{A}\cdot\mathbf{B} = \frac{1}{\mu_0}\overbrace{\int_x \nabla\cdot(\delta\mathbf{A}\times\mathbf{B})}^{=0} + \frac{1}{\mu_0}\int_x \delta\mathbf{A}(x)\cdot(\nabla\times\mathbf{B})$$

is the variation in the magnetic field energy. Setting the total variation to zero, we obtain:

$$\frac{\delta F}{\delta\mathbf{A}(x)} = -\mathbf{J}(x) + \frac{\nabla\times\mathbf{B}}{\mu_0} = 0. \tag{12.51}$$

where

$$\mathbf{J}(x) = -\frac{ie^*\hbar}{2M}\big(\psi^*\vec{\nabla}\psi - \vec{\nabla}\psi^*\,\psi\big) - \frac{e^{*2}}{M}|\psi|^2\mathbf{A}. \tag{12.52}$$

is the supercurrent density. In this way, we have rederived Ampère's equation, where the current density takes the well-known form of a probability current in the Schrodinger equation. However, $\psi(x)$ now assumes a macroscopic, physical significance - it is literally, the "macroscopic wavefunction" of the superconducting condensate. We will shortly see how Eq. (12.51) leads to the Meissner effect.

To take variations with respect to ψ, it is useful to first integrate by parts, writing

$$F_\psi = \int_x \frac{\hbar^2}{2M}\psi^*(-i\nabla - \frac{e^*}{\hbar}\mathbf{A})^2\psi + r\psi^*\psi + \frac{u}{2}(\psi^*\psi)^2\Big]. \tag{12.53}$$

[7] The variation of F_{EM} is tricky. We can carry it out using index notation to integrate δF_{EM} by parts as follows:

$$\begin{aligned}\delta F_{EM} &= \frac{1}{\mu_0}\int_x \epsilon_{abc}(\nabla_b\delta A_c)B_a = \frac{1}{\mu_0}\int_x \overbrace{\epsilon_{abc}}^{=-\epsilon_{cba}}\Big[\underbrace{\nabla_b(\delta A_c B_a)}_{0} - \delta A_c\nabla_b B_a\Big]\\ &= \frac{1}{\mu_0}\int_x \delta A_c(x)\epsilon_{cba}\nabla_b B_a = \frac{1}{\mu_0}\int_x \delta\mathbf{A}(x)\cdot(\nabla\times\mathbf{B})\end{aligned} \tag{12.50}$$

where we have set total derivative terms to zero.

If we now take variations with respect to ψ^* and ψ, we obtain

$$\delta F = \int d^dx \left(\delta\psi^*(x)\left[\frac{\hbar^2}{2M}(-i\nabla - \frac{e^*}{\hbar}\mathbf{A})^2\psi(x) + r\psi(x) + u|\psi(x)|^2\psi(x)\right] + \text{H.c}\right)$$

implying that

$$-\frac{\hbar^2}{2M}(\nabla - i\frac{e^*}{\hbar}\mathbf{A})^2\psi(x) + r\psi(x) + u|\psi(x)|^2\psi(x) = 0. \tag{12.54}$$

This "non-linear Schroedinger equation" is almost identical to (12.17) obtained for an Ising order parameter, but here $\nabla^2 \to (\nabla - i\frac{q}{\hbar}\mathbf{A})^2$ to incorporate the gauge invariance and $\psi^3 \to |\psi|^2\psi$ takes account of the complex order parameter. We will shortly see how this equation can be used to determine the surface tension σ_{sn} of a drop of superconducting fluid.

12.5.3 The Meissner Effect

We now examine how a superconductor behaves in the presence of a magnetic field. It is useful to write the supercurrent (12.52)

$$\mathbf{J}(x) = -\frac{ie^*\hbar}{2M}\left(\psi^*\vec{\nabla}\psi - \text{H.c}\right) - \frac{e^{*2}}{M}|\psi|^2\mathbf{A}$$

in terms of the amplitude and phase of the order parameter $\psi = |\psi|e^{i\phi}$ (c.f. 12.36). The derivative term $\psi^*\nabla\psi$ can be re-written

$$\psi^*\nabla\psi = |\psi|e^{-i\phi}\vec{\nabla}(|\psi|e^{i\phi}) = i|\psi|^2\vec{\nabla}\phi + |\psi|\vec{\nabla}|\psi|,$$

so that the term $\psi^*\nabla\psi - \text{H.c} = 2i|\psi|^2\nabla\phi$ and hence

$$\begin{aligned}\mathbf{J}(x) &= \frac{e^*\hbar}{M}|\psi|^2\nabla\phi - \frac{e^{*2}}{M}|\psi|^2\mathbf{A} \\ &= e^*n_s\overbrace{\frac{\hbar}{M}\left(\vec{\nabla}\phi - \frac{e^*}{\hbar}\mathbf{A}\right)}^{\mathbf{v}_s} = e^*n_s\mathbf{v}_s\end{aligned} \tag{12.55}$$

where we have replaced $|\psi|^2 = n_s$ and identified

$$\mathbf{v}_s = \frac{\hbar}{M}\left(\nabla\phi - \frac{e^*}{\hbar}\mathbf{A}\right). \tag{12.56}$$

as the superfluid velocity. Note that in contrast with (12.39), either a twist in the phase, or an external vector potential can promote a superflow. Under a gauge transformation, $\phi \to \phi + \alpha$, $\mathbf{A} \to \mathbf{A} + \frac{\hbar}{e^*}\nabla\alpha$, this combination is gauge-invariant. Written out explicitly, Ampéres equation then becomes

$$\nabla\times\mathbf{B} = -\mu_0\frac{n_se^{*2}}{M}\left(\mathbf{A} - \frac{\hbar}{e^*}\nabla\phi\right) \tag{12.57}$$

If we take the curl of this expression (assuming n_s is constant), we obtain

$$\nabla\times(\nabla\times\mathbf{B}) = \mu_0\nabla\times\mathbf{J} = -\frac{\mu_0n_se^{*2}}{M}\mathbf{B} \tag{12.58}$$

where we have used the identity $\nabla\times\nabla\phi = 0$ to eliminate the phase gradient. But $\nabla\times(\nabla\times\mathbf{B}) = \nabla(\nabla\cdot\mathbf{B}) - \nabla^2\mathbf{B} = -\nabla^2\mathbf{B}$, since $\nabla\cdot\mathbf{B} = 0$, so that

$$\boxed{\begin{aligned}\nabla^2\mathbf{B} &= \frac{1}{\lambda_L^2}\mathbf{B}, \qquad \textbf{Meissner Effect} \\ \frac{1}{\lambda_L^2} &= \frac{\mu_0n_se^{*2}}{M}\end{aligned}} \tag{12.59}$$

This equation, first derived by Fritz London on phenomenological grounds[13], expresses the astonishing property that magnetic fields are actively expelled from superconductors. The only uniform solutions that are possible are

$$\begin{aligned}\mathbf{B} = 0, n_s > 0, &\quad \text{superconductor} \\ \mathbf{B} \neq 0, n_s = 0, &\quad \text{normal state}\end{aligned} \tag{12.60}$$

One dimensional solutions to the London equation $\nabla^2B = B/\lambda_L^2$ take the form $B \sim B_0e^{-\frac{x}{\lambda_L}}$, showing that near the surface of a superconductor, magnetic fields only penetrate a distance depth λ_L into the condensate. The persistent supercurrents that screen the field out of the superconductor lie within this thin shell on the surface.

As we shall see however, in the class of type II superconductors, where the coherence length is small compared with the penetration depth ($\xi < \lambda_L/\sqrt{2}$), magnetic fields can penetrate the superconductor in a non-uniform way as vortices.

Lastly, note that in a superconductor, where $M = 2m_e$ and $e^* = 2e$ are the mass and charge of the Cooper pair respectively, while $n_s = \frac{1}{2}n_e$ is half the concentration of electrons in the condensate,

$$\frac{n_se^{*2}}{M} = \frac{\frac{1}{2}n_e4e^2}{2m_e} = \frac{n_ee^2}{m}$$

so the expression for the penetration depth has the same form when written in terms of the charge and mass of the electron.

$$\frac{1}{\lambda_L^2} = \mu_0\frac{n_ee^2}{m}$$

The critical field H_c

In a medium that is immersed in an external field, we can divide the magnetic field into an "external" magnetizing field $\mathbf{H}$ and the magnetization $\mathbf{M}$. In SI units,

$$\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M})$$

where $\mathbf{j}_{ext} = \nabla\times\mathbf{H}$ is the current density in the external coils and $\mathbf{j}_{int} = \nabla\times\mathbf{M}$ are the internal currents of the material: in a superconductor, these are the supercurrents. Now the ratio $\chi = M/H$, is the magnetic susceptibility. Since the magnetic field $\mathbf{B} = \mu_0(\mathbf{M}+\mathbf{H})$ vanishes inside a superconductor, this implies $\mathbf{M} = -\mathbf{H}$, so that [8]

$$\chi_{SC} = -1. \qquad \textbf{Perfect diamagnet}.$$

In other words, superconductors are perfect diamagnets, in which shielding supercurrents $J_{int} = \nabla\times\mathbf{M}$ provide a perfect Faraday cage to screen out the magnetic field from the interior of the superconductor.

In a superconductor, $F = F_\psi + F_{EM}$ is a sum of two terms, where $\delta F_\psi/\delta\mathbf{B}(x) = -\mathbf{M}(x)$ is the magnetization induced by the supercurrents while $\delta F_{EM}/\delta\mathbf{B}(x) = {\mu_0}^{-1}\mathbf{B}(x)$ is the magnetic field. Adding these terms together,

$$\frac{\delta F}{\delta\mathbf{B}(x)} = -\mathbf{M}(x) + \frac{1}{\mu_0}\mathbf{B}(x) = \mathbf{H}$$

Now the magnetizing field $\mathbf{H}$ is determined by the external coils, and can be taken to be constant over the scale of the coherence and penetration depth. Since it is the external field $\mathbf{H}$ that is fixed, it is more convenient to use the Gibb's free energy

$$G[\mathbf{H},\psi] = F[\mathbf{B},\psi] - \int d^3x\mathbf{B}(x)\cdot\mathbf{H}$$

which is a functional of the external field $\mathbf{H}$ and independent of the $B-$ field ($\delta G/\delta\mathbf{B} = 0$). The second term describes the work done by the coils in producing the constant external field. This is analogous to setting $G[P] = F[V] + PV$ to include the work PV done by a piston to maintain a fluid at constant pressure. In a uniform superconductor,

$$g = \frac{G}{V} = r|\psi|^2 + \frac{u}{2}|\psi|^4 + \frac{B^2}{2\mu_0} - BH$$

In the normal state, $\psi = 0$, $B = \mu_0 H$, so that

$$g_n = -\frac{B^2}{2\mu_0}$$

whereas in the superconducting state, $B = 0$, and $|\psi| = \psi_0 = \sqrt{-r/u}$, so that

$$g_{sc} = r\psi_0^2 + \frac{u}{2}\psi_0^4 = -\frac{r^2}{2u}$$

Clearly, if $g_{sc} < g_n$, i.e, if

$$B < B_c = \sqrt{\mu_0\frac{r^2}{u}} \qquad \text{critical field} \qquad (12.61)$$

the superconductor is thermodynamically stable. The free energy density of the superconductor can then be written

$$g_{sc} = -\frac{r^2}{2u} = -\frac{1}{2\mu_0}B_c^2$$

[8] Most older texts use Gaussian units, for which $\chi_{SC} = -\frac{1}{4\pi}$ in a superconductor. In Gaussian units $\mathbf{B} = \mathbf{H} + 4\pi\mathbf{M} = (1+4\pi\chi)\mathbf{H}$. If $\mathbf{B} = \mathbf{0}$, this implies that $\chi^{SC} = -\frac{1}{4\pi}$ in Gaussian units.

Surface energy of a superconductor.

When $B = B_c$, the free energy density of the normal state and the superconductor are identical, and so the two phases can co-exist. The interface between the degenerate superconductor and normal is a domain wall, where the Gibb's energy per unit energy defines the surface energy

$$\Delta G/A = \sigma_{sn}$$

where A is the area of the interface. At the interface the superconducting order parameter and the magnetic field decay away to zero over length scales of order the coherence length ξ and penetration depth λ_L, respectively, as illustrated below.

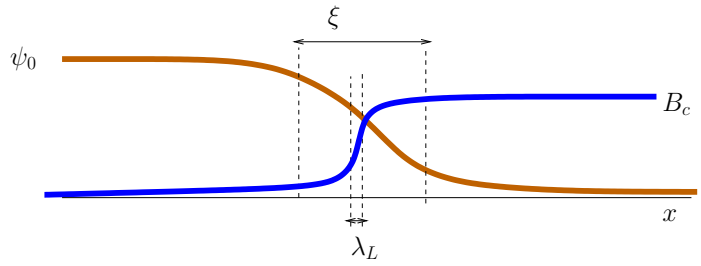

Figure 12.7: Schematic illustrating a superconductor-normal metal domain wall in a type I superconductor, where $\xi >> \lambda_L$.

The surface tension σ_{sn} (surface energy) σ_{ns} of the domain wall between the superconductor and normal phase has a profound influence on the macroscopic behavior of a superconductor. The key parameter which controls the surface tension is the ratio of the magnetic penetration to the coherence length,

$$\kappa = \frac{\lambda_L}{\xi}, \qquad \textbf{Ginzburg Landau parameter.}$$

There are two types of superconductor:

1. $\kappa < \frac{1}{\sqrt{2}}$ **Type I superconductors**, with a positive domain wall energy. In type I superconductors, magnetic fields are vigorously excluded from the material by a thin surface layer of screening currents (Fig 12.8(a)). At $H = H_c$ there is a first order transition into the normal state.

2. $\kappa > \frac{1}{\sqrt{2}}$ **Type II superconductors**, with a negative surface tension ($\sigma_{sn} < 0$). In type II superconductors, the surface layer of screening currents is smeared out on the scale of the coherence length, and the magnetic field penetrates much further into the superconductor (Fig 12.8(b)). In type II superconductors, there are now two critical fields, an "upper" critical field

$H_{c2} > H_c$ and a lower critical field $H_{c1} < H_c$. Between these two fields, $H_{c1} < H < H_{c2}$ the magnetic field penetrates the bulk, forming vortices in which the high energy of the normal core is offset by the negative surface energy of the layer of screening currents.

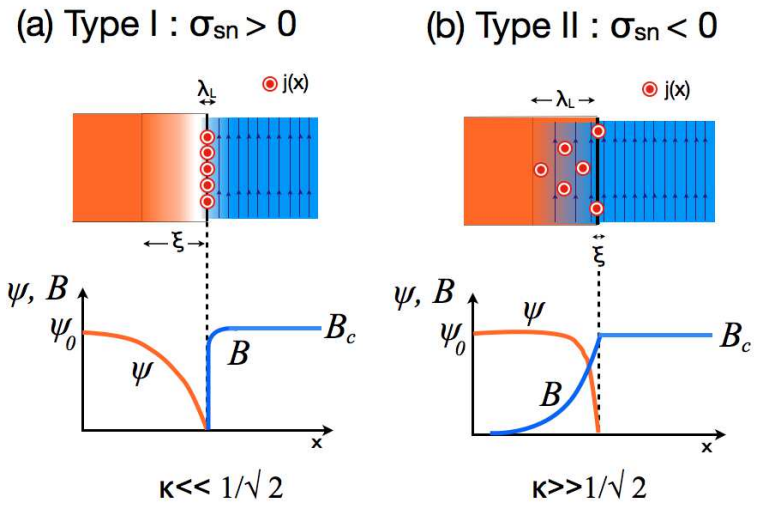

Figure 12.8: Superconductor-normal domain wall in type I and type II superconductors. (a) For $\kappa = \frac{\lambda_L}{\xi} < \frac{1}{\sqrt{2}}$, the superconductor is a type *I* superconductor. In the limit $\kappa \to 0$ illustrated here, the magnetic field drops precipitously to zero at $x = 0$. In the extreme type I limit $\kappa >> 1/\sqrt{2}$, the magnetic field and the screening currents extend a distance of $\lambda_L >> \xi$ into the superconductor.

The domain wall energy between a superconductor and a metal at $H = H_c$ is the excess energy associated with a departure from uniformity:

$$\sigma_{ns} = \frac{1}{A}\int d^3x\Big[\frac{\hbar^2}{2M}\Big|(\nabla - \frac{ie^*}{\hbar}\mathbf{A})\psi\Big|^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4 + \frac{B^2}{2\mu_0} - \mathbf{B}\cdot\mathbf{H}_c - g_{sc}\Big] \tag{12.62}$$

Inserting $H_c = B_c/\mu_0$ and $g_{sc} = -\frac{B_c^2}{2\mu_0}$, we see that the last three terms can be combined into one, to obtain

$$\sigma_{ns} = \frac{1}{A}\int d^3x\Big[\frac{\hbar^2}{2M}\Big|(\nabla - \frac{ie^*}{\hbar}\mathbf{A})\psi\Big|^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4 + \frac{(B-B_c)^2}{2\mu_0}\Big] \tag{12.63}$$

By imposing the condition of stationarity, it is straightforward to show (see example 12.6) that the domain wall energy of a domain in the y-z plane can be cast into the compact form

$$\sigma_{sn} = \frac{B_c^2}{2\mu_0}\int_{-\infty}^{\infty} dx\left[\left(\frac{B(x)}{B_c} - 1\right)^2 - \left(\frac{\psi(x)}{\psi_0}\right)^4\right]. \tag{12.64}$$

This compact form for the surface tension of a superconductor can be loosely interpreted as the difference of field and condensation energy

$$\sigma_{sn} = \int_{-\infty}^{\infty} dx\,[\text{field energy} - \text{condensation energy}]$$

In the superconductor at the critical field, these two terms terms directly cancel one another whereas in the normal metal both terms are zero. It is the imperfect balance of these two energy terms at the interface that creates a non-zero surface tension. In a type I superconductor, the healing length ξ for the order parameter is long so the condensation energy fails to compensate for the field energy generating a positive surface tension. By contrast, in a type II superconductor, the healing length for the magnetic field λ_L is large so the field energy fails to compensate for the condensation energy leading to a negative surface tension. In fact, within Ginzburg Landau theory, the surface tension vanishes at $\kappa = 1/\sqrt{2}$ (see example 12.7), so $\kappa = 1/\sqrt{2}$ is the dividing line between the two classes of superconductor. Summarizing:

$$\begin{array}{lllll} \textbf{Type I:} & (\kappa < 1/\sqrt{2}) & \text{Interface condensation energy} < \text{field energy} & \sigma_{sn} > 0 \\ \textbf{Type II:} & (\kappa > 1/\sqrt{2}) & \text{Interface field energy} < \text{condensation energy} & \sigma_{sn} < 0 \end{array} \tag{12.65}$$

One of the most dramatic effects of a negative surface tension, is the stabilization of non-uniform superconducting states at fields over a wide range of fields between B_{c1} and B_{c2}, where $B_{c2} = \sqrt{2}\kappa B_c$ is the "upper critical field", and $B_{c1} \sim B_c/(\sqrt{2}\kappa)$ is the "lower critical field".

Let us estimate the surface tension in extreme type I and type II superconductors (Fig. 12.8). In the former, where $\lambda_L << \xi$, the length scale over which the magnetic field varies is negligible relative to the coherence length(see Fig. 12.8(a)), so that the magnetic field can be approximated by a step function

$$B(x) = B_c\theta(x), \qquad \textbf{Extreme type I}.$$

For $x > 0$, $B(x) = B_c$ is constant, which implies that $B'' \propto \psi^2 B_c = 0$, so that $\psi(x) = 0$ for $x \geq 0$. For $x < 0$, on the superconducting side of the domain wall, $\mathbf{B} = \mathbf{A} = \mathbf{0}$ and in the absence of a field, the evolution equation for ψ is identical to an Ising kink treated in section (12.3.1), for which the solution is $\psi/\psi_0 = \tanh(x/(\sqrt{2}\xi))$. Substituting into (12.64), the surface tension is then

$$\sigma^{\rm I}_{sn} = \frac{B_c^2}{2\mu_0}\int_{-\infty}^{0} dx\left[1 - \tanh(x/(\sqrt{2}\xi))^4\right] = \frac{B_c^2}{2\mu_0}\times 1.89\xi \tag{12.66}$$

For an extreme type II superconductor, the situation is reversed: now the longest length-scale is the penetration depth. Unfortunately, since the vector potential modifies the equilibrium magnitude of the order parameter, λ_L sets the decay length of *both* the field and the order parameter. Let us

nevertheless estimate the surface tension by treating the order parameter as a step function $\psi(x) \sim \psi_0\theta(-x)$. In this case, $A'' = \frac{1}{\lambda_L^2}(\psi/\psi_0)^2 A$, so that

$$B(x) = B_c \times \begin{cases} e^{x/\lambda_L} & (x<0) \\ 1 & (x>0) \end{cases} \tag{12.67}$$

Substituting into (12.76), this then gives

$$\sigma_{sn}^{\rm II} \approx \frac{B_c^2}{2\mu_0}\int_{-\infty}^{0} dx[(e^{x/\lambda_L}-1)^2 - 1] = -\frac{B_c^2}{2\mu_0}\times\frac{3}{2}\lambda_L \tag{12.68}$$

showing that at large κ, the surface tension becomes negative. The result of a more detailed calculation (example 12.8) replaces the factor of 3/2 by $(8/3)(\sqrt{2}-1) = 1.1045$ [14].

Summarizing the results of a detailed Landau Ginzburg calculation,

$$\sigma_{ns} = \frac{B_c^2}{2\mu_0}\times\begin{cases} 1.89\xi & \text{(extreme type I)} \\ -1.10\lambda_L & \text{(extreme type II)} \end{cases}$$

Example 12.6: Calculate the domain wall energy per unit area σ_{ns} of a superconducting-normal interface lying in the $y-z$ plane, and show that it can be written

$$\sigma_{sn} = \frac{B_c^2}{2\mu_0}\int_{-\infty}^{\infty} dx\left[\left(\frac{B(x)}{B_c}-1\right)^2 - \left(\frac{\psi(x)}{\psi_0}\right)^4\right]. \tag{12.69}$$

Solution: Consider a domain wall in the $y-z$ plane separating a superconductor at $x<0$ from a metal at $x>0$, immersed in a magnetic field along the $z-axis$. Let us take

$$\mathbf{A}(x) = (0, A(x), 0), \qquad \mathbf{B}(x) = (0, 0, A'(x)),$$

seeking a domain wall solution in which $\psi(x)$ is real. Our boundary conditions are then

$$(\psi(x),\ A(x)) = \begin{cases} (\psi_0, 0) & (x\to-\infty) \\ (0, xB_c) & (x\to+\infty) \end{cases} \tag{12.70}$$

The domain wall energy is then

$$\sigma_{sn} = \frac{G}{A} = \int dx\left[\frac{\hbar^2}{2M}\left\{\left(\frac{d\psi}{dx}\right)^2 + \frac{e^{*2}A^2}{\hbar^2}\psi^2\right\} + r\psi^2 + \frac{u}{2}\psi^4 + \frac{(B-B_c)^2}{2\mu_0}\right] \tag{12.71}$$

Notice that there are no terms linear in $d\psi/dx$, because the vector potential and the gradient of the order parameter are orthgonal ($\nabla\psi\cdot\mathbf{A}=0$). Let us rescale the x co-ordinate in units of the penetration length, the order parameter in units of ψ_0 and the magnetic field in units of the critical field, as follows:

$$\tilde{x} = \frac{x}{\lambda_L}, \qquad \tilde{\psi} = \frac{\psi}{\psi_0}, \qquad \tilde{A} = \frac{A}{B_c\lambda_L}, \qquad \tilde{B} = \frac{B}{B_c} = \frac{d\tilde{A}}{d\tilde{x}} \equiv \tilde{A}'.$$

In these rescaled variables, the Gibb's free energy becomes

$$\sigma_{sn} = \frac{B_c^2\lambda_L}{2\mu_0}\int dx\left[\frac{2\psi'^2}{\kappa^2} + A^2\psi^2 + \left((\psi^2-1)^2-1\right) + (A'-1)^2\right]. \tag{12.72}$$

where for clarity, we have now dropped the tildes. The rescaled boundary conditions are $(\psi, A)\to(1,0)$ in the superconductor at $x<<0$, and $(\psi, A)\to(0, x)$ deep inside the metal at $x>>0$.

Taking variations with respect to ψ gives

$$-\frac{\psi''}{\kappa^2} + \frac{1}{2}A^2\psi + (\psi^2-1)\psi = 0 \tag{12.73}$$

while taking variations with respect to A gives the dimensionless London equation

$$A\psi^2 - A'' = 0 \tag{12.74}$$

Integrating by parts to replace $(\psi')^2 \to -\psi\psi''$ in (12.72), we obtain

$$\sigma_{sn} = \frac{B_c^2\lambda_L}{2\mu_0}\int dx\overbrace{\left[\frac{2\psi\psi''}{\kappa^2}+A^2\psi^2+\left((\psi^2-1)^2-1\right)\right]}^{-A^2\psi^2-2(\psi^2-1)\psi^2} + (A'-1)^2\Big] \tag{12.75}$$

where we have used (12.73) to elimiate ψ''. Cancelling the $A^2\psi^2$ and ψ^2 terms in (12.75), we can then write the surface tension in the compact form

$$\sigma_{sn} = \frac{B_c^2\lambda_L}{2\mu_0}\int_{-\infty}^{\infty} dx\left[(A'(x)-1)^2 - \psi(x)^4\right]. \tag{12.76}$$

Restoring $x\to\frac{x}{\lambda_L}$, $A'(x)\to\frac{B(x)}{B_c}$ and $\psi(x)\to\frac{\psi(x)}{\psi_0}$, we obtain (12.64).

Example 12.7: Show that the domain wall energy changes sign at $\kappa = 1/\sqrt{2}$.

Solution: Using equation (12.76), we see that in the special case where the surface tension $\sigma_{sn}=0$, is zero, it follows that

$$A'(x) = 1 \mp \psi(x)^2$$

where we select the upper choice of signs to give a physical solution where the field is reduced inside the superconductor ($A'<1$). Taking the second derivative, gives $A'' = -2\psi\psi'$. But since $A'' = \psi^2 A$, it follows that $\psi' = -\frac{1}{2}A\psi$. Now we can derive an alternative expression for ψ' by integrating the second order equation (12.74). By multiplying (12.73) by $4\psi'$, using (12.74) we can rewrite (12.73) as a total derivative

$$\frac{d}{dx}\left[-\frac{2}{\kappa^2}(\psi')^2 + A^2\psi^2 + (\psi^2-1)^2 - A'^2\right] = 0$$

from which we deduce that

$$-\frac{2}{\kappa^2}(\psi')^2 + A^2\psi^2 + (\psi^2-1)^2 - A'^2 = \text{constant} = 0 \tag{12.77}$$

is constant across the domain, where the value of the constant is obtained by placing $\psi = 1$, $A = A' = 0$ on the superconducting side of the domain. Substituting $A' = (1-\psi^2)$, the last two terms cancel. Finally, putting $(\psi')^2 = \frac{1}{4}(A\psi)^2$, we obtain

$$\left(1 - \frac{1}{2\kappa^2}\right)(A\psi)^2 = 0, \tag{12.78}$$

showing that $\kappa_c = 1/\sqrt{2}$ is the critical value where the surface tension drops to zero.

Example 12.8: Using the results of the example 13.6, show that within Landau Ginzburg theory, the surface tension of an extreme type II superconductor is [14]

$$\sigma_{ns} = -\frac{B_c^2}{2\mu_0} \times \frac{8}{3}(\sqrt{2}-1)\lambda_L \approx -\frac{B_c^2}{2\mu_0} \times 1.10\lambda_L$$

Solution: We start with equations (12.73) and (12.74)

$$\frac{\psi''}{\kappa^2} + \frac{1}{2}A^2\psi + (\psi^2-1)\psi = 0 \tag{12.79}$$

$$A\psi^2 - A'' = 0 \tag{12.80}$$

For an extreme type II superconductor, $\kappa >> 1$ allowing us to neglect the derivative term in the first equation. There are then two solutions:

$$\begin{aligned} \psi^2 &= 1 - \tfrac{1}{2}A^2, && (x<0) \\ \psi &= 0, \qquad A = x + \sqrt{2} && (x>0) \end{aligned} \tag{12.81}$$

For $(x<0)$, substituting into (12.80), we then obtain

$$A(1 - A^2/2) = A'' \tag{12.82}$$

Multiplying both sides by the integrating factor $2A'$, we obtain

$$\frac{d}{dx}\left(A^2(1-A^2/4)\right) = \frac{d}{dx}(A')^2$$

or $A^2(1-A^2/4) = (A')^2 + \text{cons}$, where the integration constant vanishes because A and A' both go to zero as $x \to -\infty$, so that

$$A' = A\sqrt{1 - A^2/4}, \qquad (x<0) \tag{12.83}$$

Now using (12.81) in (12.76), the surface tension is

$$\begin{aligned} \sigma_{sn} &= \frac{B_c^2\lambda_L}{2\mu_0} \times I \\ I &= \int_{-\infty}^{0} \left[(A'-1)^2 - (1-A^2/2)^2\right] dx \end{aligned} \tag{12.84}$$

Substituting for A' using (12.83) then gives

$$\begin{aligned} I &= \int_{-\infty}^{0} \left[(A\sqrt{1-A^2/4}-1)^2 - (1-A^2/2)^2\right] dx \\ &= \int_{-\infty}^{0} \left[2A^2(1-A^2/4) - 2A\sqrt{1-A^2/4}\right] dx \\ &= \int_{-\infty}^{0} \left[2(A'-1)\right] A' dx \\ &= \int_{0}^{\sqrt{2}} 2\left[(A\sqrt{1-A^2/4}-1)\right] dA = -\frac{8}{3}\left(\sqrt{2}-1\right) \approx -1.1045 \end{aligned} \tag{12.85}$$

where we have used the fact that $\psi = 0$, $A = \sqrt{2}$ at $x = 0$. It follows that in the extreme type II superconductor

$$\sigma_{sn} = -\frac{B_c^2}{2\mu_0} \times (1.10\lambda_L).$$

12.5.4 Vortices, Flux quanta and type-II superconductors.

Once $H > H_{c1}$, type II superconductors support the formation of superconducing vortices.

In a neutral superfluid, a superconducting vortex is a line defect around which the phase of the order parameter precesses by 2π, or a multiple of 2π. In section (12.4.3), we saw that this gave rise to a quantization of circulation. In a superconducting vortex, the rotating electric currents give rise to a trapped magnetic flux, quantized in units of the superconducting flux quantum

$$\Phi_0 = \frac{h}{e^*} \equiv \frac{h}{2e}.$$

This quantization of magnetic flux we predicted by London and Onsager[13, 15].

To understand flux quantization, it is instructive to contrast a neutral superfluid with a superconducting vortex (see Fig. 12.9). In a neutral superfluid, the superfluid velocity is uniquely dictated by the gradient of the phase, $\mathbf{v}_s = \frac{\hbar}{M}\vec{\nabla}\phi$, so around a vortex, the superfluid velocity decays as $1/r$ ($v_s = n \times \frac{h}{Mr}$). Around a superconducting vortex, the superfluid velocity contains an additional contribution from the vector potential

$$\mathbf{v}_s = \frac{\hbar}{M}\vec{\nabla}\phi - \frac{e^*}{M}\mathbf{A}.$$

In the presence of a magnetic field, this term compensates for the phase gradient, lowering the supercurrent velocity and reducing the overall kinetic energy of the vortex. On distances larger

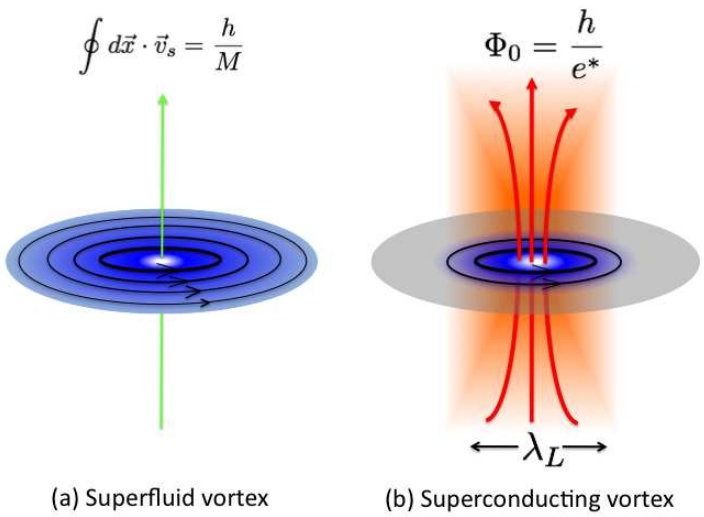

Figure 12.9: Contrasting (a) a vortex in a neutral superfluid with (b) a vortex in a superconductor, where each unit of quantized circulation binds one quanta of magnetic flux.

than the penetration depth λ_L the vector potential and the phase gradient almost completely cancel one-another, leading to a supercurrent that decays exponentially with radius $v_{sc} \propto e^{-r/\lambda_L}$.

If we integrate the circulation around a vortex, we find

$$\omega = \oint d\mathbf{x}\cdot\mathbf{v}_s = \frac{\hbar}{M}\overbrace{\oint d\mathbf{x}\cdot\vec{\nabla}\phi}^{\Delta\phi=2\pi n} - \frac{e^*}{M}\overbrace{\oint d\mathbf{x}\cdot\mathbf{A}}^{\Phi} \tag{12.86}$$

where we have identified $\oint d\mathbf{x}\cdot\vec{\nabla}\phi = 2\pi\times n$ as the total change in phase around the vortex, while $\oint d\mathbf{x}\cdot\mathbf{A} = \int \mathbf{B}\cdot d\mathbf{S} = \Phi$ is the magnetic flux contained within the loop, so that

$$\omega = n\frac{h}{M} - \frac{e^*\Phi}{M}.$$

In this way, we see that the presence of bound magnetic flux reduces the total circulation. At large distances, energetics favor a reduction of the circulation to zero, $\lim_{R\to\infty}\omega = 0$, so that around a large loop

$$0 = n\frac{h}{M} - \frac{e^*\Phi}{M}$$

or

$$\Phi = n\left(\frac{h}{e^*}\right) = n\Phi_0 \tag{12.87}$$

where $\Phi_0 = \frac{h}{e^*}$ is the quantum of flux. In this way, each quantum of circulation generates a bound quantum of magnetic flux. The lowest energy vortex contains a single flux, as illustrated in Fig. 12.9 A simple realization of this situation occurs in a hollow superconducting cylinder (Fig. 12.10). In its lowest energy state, where no supercurrent flows around the cylinder, the magnetic flux trapped inside the cylinder is quantized. If an external magnetic field is is applied to the cylinder, and then later removed, the cylinder is found to trap flux in units of the flux quantum $\Phi_0 = \frac{h}{2e}$, [16, 17], providing a direct confirmation of the charge of the Cooper pair

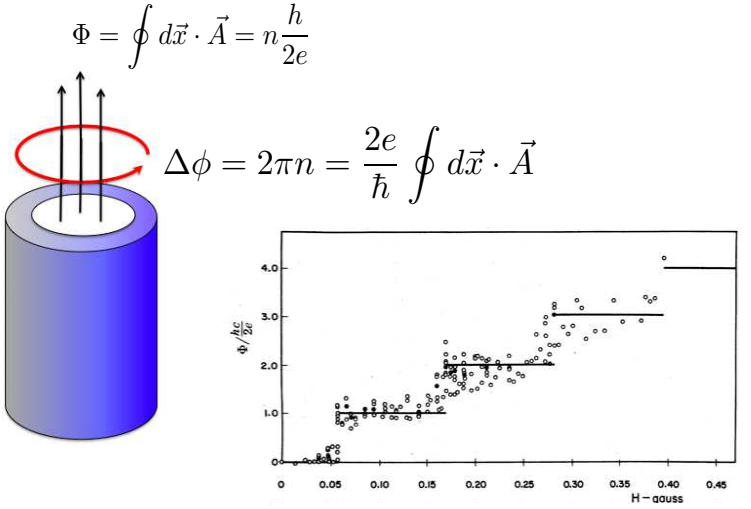

Figure 12.10: Flux quantization inside a cylinder. In the lowest energy configuration, with no supercurrent in the cylinder walls, the $\Delta\phi = 2\pi n$ twist in the phase of the order parameter around the cylinder is compensated by a quantized circulation of the vector potential, giving rise to a quantized flux. The inset shows quantized flux measured in reference [16].

In thermodynamic equilibrium, vortices penetrate a type II superconductor provided the applied field H lies between the upper and lower critical fields H_{c2} and H_{c1} respectively. In an extreme type II superconductor, H_{c2} and H_{c1} differ from H_c by a factor of $\kappa = \frac{\lambda_L}{\xi}$:

$$H_{c1} \sim \frac{H_c \ln\kappa}{\sqrt{2}\kappa} \qquad (\kappa >> 1) \tag{12.88}$$

$$H_{c2} = \sqrt{2}\kappa H_c. \tag{12.89}$$

Below H_{c1} and above H_{c2} the system is uniformly superconducting and normal respectively. In between, fluxoids self-organize themselves into an ordered triangular lattice, called the Abrikosov Flux Lattice. Thus H_{c1} is the first field at which it becomes energetically advantageous to add a vortex to the uniform super conductor, whereas H_{c2} is the largest field at which a non-uniform superconducting solution is still stable.

For an extreme type II superconductor, H_{c1} can be made calculating the field at which the Gibb's Free energy of a vortex

$$\begin{aligned}\Delta G_V &= \epsilon_V L - \mathbf{H}\cdot\int d^3x \mathbf{B}(x) \\ &= \epsilon_V L - H\Phi_0 L,\end{aligned} \tag{12.90}$$

becomes negative. Here L is the length of the vortex and ϵ_V is the vortex energy per unit length. For an extreme type II superconductor, this energy is roughly equal to the lost condensation energy of the core. Assuming the core to have a radius ξ, this is

$$\epsilon_V \sim \frac{r^2}{2u}\times\pi\xi^2 = \frac{B_c^2}{2\mu_0}\pi\xi^2.$$

Vortices will start to enter the condensate when $\Delta G_V < 0$, i.e when

$$H_{c1}\Phi_0 \sim \frac{B_c^2}{2\mu_0}\times\pi\xi^2.$$

Putting $H_{c1} = B_{c1}/\mu_0$, and estimating the area over which the magnetic field is spread to be $\pi\lambda_L^2$, so that the total flux, $\Phi_0 = B_{c1}\times\pi\lambda_L^2$, we obtain

$$\frac{H_{c1}}{H_c} \sim \frac{1}{\kappa}$$

so that $H_{c1} << H_c$ for an extreme type II superconductor. A more detailed calculation gives the answer quoted in (12.88).

To calculate H_{c2}, consider a metal in which the applied field is gradually reduced from a high field. H_{c2} will be the field at which the first non-uniform superconducting solution becomes possible. Non uniform solutions of the order parameter satisfy the non-linear Schroedinger equation (12.54),

$$\frac{\hbar^2}{2M}(-i\nabla - \frac{e^*}{\hbar}\mathbf{A})^2\psi(x) + r\psi(x) + u|\psi(x)|^2\psi(x) = 0. \tag{12.91}$$

Since the developing superconducting instability will have a very small amplitude, we can ignore the cubic term. Choosing $\mathbf{A} = (0, 0, Bx)$, let us now seek solutions of ψ that depend only on x, so that

$$-\frac{\hbar^2}{2M}\psi'' + \frac{1}{2}m\omega_c^2\psi = -r\psi(x). \tag{12.92}$$

where $\omega_c = \frac{e^*B}{M}$. This as the time-independent Schroedinger equation for a harmonic oscillator with energy $E = -r$. Since the smallest energy eigenvalue is $E = \frac{1}{2}\hbar\omega_c$, it follows that $-r = \frac{1}{2}\hbar\omega_c$. Now according to (12.27), the coherence length is given by $\xi^2 = \frac{\hbar^2}{2M|r|}$, so that $|r| = \frac{\hbar^2}{2M\xi^2} = \hbar\frac{e^*B_{c2}}{M}$, so that

$$2\pi B_{c2}\xi^2 = \frac{h}{e^*} = \Phi_0 \tag{12.93}$$

where $\Phi_0 = \frac{h}{e^*}$ is the superconducting flux quantum. At the uppercritical field, a tube of radius ξ contains half a flux quanta, $\Phi_0/2$.

Using (12.93), the upper critical field is given by

$$B_{c2} = \frac{\hbar}{e^*\xi^2} = \frac{1}{e^*\xi}\sqrt{2M|r|}.$$

By contrast, using (12.61) and (12.49) the critical field B_c is given by

$$B_c = \sqrt{\frac{\mu_0 r^2}{u}} = \frac{1}{e^*\lambda_L}\sqrt{M|r|}$$

so that the ratio

$$\frac{B_{c2}}{B_c} = \sqrt{2}\frac{\lambda_L}{\xi} = \sqrt{2}\kappa$$

Thus provided $\kappa > \frac{1}{\sqrt{2}}$, the condition for type II superconductivity, the upper-critical field B_{c2} exceeds the thermodynamic critical field, $B_{c2} > B_c$.

12.6 Dynamical effects of broken symmetry: Anderson Higg's mechanism

One of the most dramatic effects of broken symmetry lies in its influence on gauge fields that couple to the condensate. This effect, called the "Anderson Higg's mechanism". not only lies behind the remarkable Meissner effect, but it is responsible for the short-range character of the weak nuclear force. When a gauge field couples to the long-wavelength phase modes of a charged order parameter, it absorbs the phase modes to become a massive gauge field that mediates a short range (screened) force:

gauge field + phase ⟶ massive gauge field.

Superconductivity is the simplest, and historically, the first working model of this mechanism, which today bears the name of Anderson, who first recognized its more general significance for relativistic Yang Mills theories[18], and Higg's who formulated these ideas in an action formulation [19].

In this section, we provide an introduction to the Anderson Higg's mechanism, using a simple time-dependent extension of Ginzburg Landau theory that in essence, applies the method used by Higg's[19] to the simpler case of a $U(1)$ gauge field.

12.6.1 Goldstone mode in neutral superfluids

In the ground-state, Ginzburg Landau theory can be thought of as describing the "potential energy" $V[\psi] \equiv F_{GL}[\psi]|_{T=0}$ associated with a static and slowly varying configuration of the order parameter. At scales much longer than the coherent length, amplitude fluctuations of the order parameter can be neglected, and all the physics is contained in the phase of the order parameter. For a neutral superfluid $V = \frac{1}{2}\rho_s(\nabla\phi)^2$, where ρ_s is the superfluid stiffness, given in Ginzburg Landau theory by $\rho_s = \frac{\hbar^2 n_s}{2M}$. But to determine the dynamics, we need the Lagrangian $L = T - V$ associated with slowly varying configurations of the order parameter, where T is the "kinetic" energy associated with a time-dependent field configurations. The kinetic energy can also be expanded to leading order in the time-derivatives of the phase (see exercise 13.8), so that the action governing the slow phase dynamics is

$$S = \frac{\rho_s}{2}\int dt d^3x \overbrace{\left[(\dot\phi/c^*)^2 - (\nabla\phi)^2\right]}^{\text{“}-\nabla_\mu\phi\nabla^\mu\phi\text{”}} \tag{12.94}$$

In relativistic field theory, $c^* = c$ is the speed of light, and Lorentz invariance permits the action to be simplified using a 4-vector notation $-(\nabla l_\mu\phi)^2$as shown in the brackets above. The relativistic action and the Ginzburg Landau free energy can be viewed as Minkowskii and Euclidean versions of the same energy functional:

$$\overbrace{S = -\frac{\rho_s}{2}\int d^4x(\nabla_\mu\phi)^2}^{\text{Minkowski}} \longleftrightarrow \overbrace{F = \frac{\rho_s}{2}\int d^3x(\nabla\phi)^2}^{\text{Euclidean}} \tag{12.95}$$

However, in a non-relativistic superfluid, c^* is a characteristic velocity of the condensate. For example, in a paired fermionic superfluid, such as superfluid $He-3$, $c^* = \sqrt{3}v_F$, where v_F is the Fermi velocity of the the underlying Fermi liquid. If we take variations with respect to ϕ, (integrating by parts in space-time so that $\nabla\delta\phi\nabla\phi \rightarrow -\delta\phi\nabla^2\phi$, and $\delta\dot\phi\dot\phi \rightarrow -\delta\phi\ddot\phi$), we see that ϕ satisfies the wave equation

$$\nabla^2\phi - \frac{1}{c^{*2}}\frac{\partial^2\phi}{\partial t^2} = 0 \qquad \text{Boguilubov phase mode} \quad \omega = c^*q$$

corresponding to a phase mode that propagates at a speed c^*. This mode, often called a "Boguilubov mode" is actually a special example of a Goldstone mode. The infinite wavelength limit of this mode corresponds to a simple uniform rotation of the phase, and is an example of naturally gapless mode that appears when a continuous symmetry is broken in a system governed by short-range forces.

Example 12.9: If density fluctuations $\delta n_s(x) = n_s(x) - n_s$ are included into the Hamiltonian of a superfluid, the ground-state energy is given by

$$H = \int d^3x\left[\frac{(n_s(x)-n_s)^2}{2\chi} + \frac{\rho_s}{2}(\nabla\phi)^2\right]$$

where $\chi = \partial N/\partial\mu$ is the charge susceptibility. From (see Ex. 13.5) we learned that density and phase are conjugate variables, which in the continuum satisfy Hamiltons equation that $\delta H/\delta n_s(x) = \mu(x) = -\hbar\dot\phi(x)$. Using this result, show that that the Lagrangian $L = \int d^3x\frac{\delta H}{\delta n_s(x)}\delta n_s(x) - H$ can be written in the form

$$L = \frac{\rho_s}{2}\int d^3x\left[(\dot\phi/c^*)^2 - (\nabla\phi)^2\right]$$

where $(c^*)^2 = \rho_s/(\chi\hbar^2)$.

Solution: By varying the Hamiltonian with respect to the local density, we obtain the local chemical potential of the condensate

$$\mu(x) = \frac{\delta H}{\delta n_s(x)} = \chi^{-1}\delta n_s(x). \tag{12.96}$$

By writing the condensate order parameter as $\psi(x,t) = \psi e^{i\phi(x,t)} = \psi e^{-i\frac{\mu(x)}{\hbar}t}$, we may identify $\frac{\mu(x)}{\hbar} = -\dot\phi$ as the rate of change of phase, thus from (12.96), we obtain

$$\hbar\dot\phi = -\chi^{-1}\delta n_s(x)$$

so that $(\delta n_s)^2/(2\chi) = \frac{\chi}{2}(\dot\phi)^2$ and the Lagrangian takes the form

$$L = \int d^3x(-\hbar\dot\phi\delta n_s) - H = \frac{1}{2}\int d^3x\left[\chi(\hbar\dot\phi/c^*)^2 - \rho_s(\nabla\phi)^2\right]$$

Replacing $\hbar^2\chi = \rho_s/c^{*2}$, we obtain the result.

12.6.2 Anderson Higgs mechanism

The situation is subtlely different when we consider a charged superfluid. In this case, changes in phase of the order parameter become coupled by the long-range electromagnetic forces, and this has the effect of turning them into gapped "plasmon" modes of the superflow and condensate charge density.

From Ginzburg Landau theory, we already learned that in a charge field, physical quantities, such as the supercurrent and the Ginzburg Landau free energy , depend on the the gauge invariant gradient of the phase $\nabla\phi - \frac{e^*}{\hbar}\mathbf{A}$. Since the action involves time-dependent phase configurations, it must be invariant under both space and time-dependent gauge transformations(12.45),

$$\phi \rightarrow \phi + \alpha(x,t), \qquad \mathbf{A} \rightarrow \mathbf{A} + \frac{\hbar}{e^*}\nabla\alpha, \qquad \varphi \rightarrow \varphi - \frac{\hbar}{e^*}\dot\alpha. \tag{12.97}$$

which means that time derivatives of the phase must occur in the gauge-invariant combination $\dot{\phi} + \frac{e^*}{\hbar}\varphi$, where φ is the electric potential. The action of a charged superluid now involves two terms

$$S = S_\psi + S_{EM}$$

where

$$S_\psi = \int dtd^3x \frac{\rho_s}{2}\left[\frac{1}{c^{*2}}\left(\dot{\phi} + \frac{e^*}{\hbar}\varphi\right)^2 - (\nabla\phi - \frac{e^*}{\hbar}\mathbf{A})^2\right] \tag{12.98}$$

is the gauged condensate contribution to the action and

$$S_{EM} = \frac{1}{2\mu_0}\int dtd^3x\left[\left(\frac{E}{c}\right)^2 - B^2\right] \tag{12.99}$$

is the electromagnetic Lagrangian, where $\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi$ and $\mathbf{B} = \nabla\times\mathbf{A}$ are the electric and magnetic field respectively.

The remarkable thing, is that since the scalar and vector potential always occur in the same gauge invariant combination with the phase gradients, we can redefine the electromagnetic fields to completely absorb the phase gradients as follows:

$$\mathbf{A}' = \mathbf{A} - \frac{\hbar}{e^*}\nabla\phi, \quad \varphi' = \varphi + \frac{\hbar}{e^*}\dot{\phi}, \qquad\qquad (A^\mu \to \frac{\hbar}{e^*}\nabla^\mu\varphi).$$

Notice that in (12.98), the vector potential, which we associate with transverse electromagnetic waves, becomes coupled to gradients of the phase, which are longitudinal in character. The sum of the phase gradient and the vector potential creates a field with both longitudinal and transverse character. In terms of the new fields, the action becomes

$$S = \int dtd^3x\Big\{\overbrace{\frac{1}{2\mu_0\lambda_L^2}\left[\left(\frac{\varphi}{c^*}\right)^2 - \mathbf{A}^2\right]}^{L_\psi} + \overbrace{\frac{1}{2\mu_0}\left[\left(\frac{E}{c}\right)^2 - B^2\right]}^{L_{EM}}\Big\}. \tag{12.100}$$

where $1/(\mu_0\lambda_L^2) = (\rho_s e^{*2})/(\hbar^2) = n_s e^{*2}/M$ defines the London penetration depth and we have dropped the primes on φ and $\mathbf{A}$ in subsequent equations.

Amazingly, by absorbing the phase of the order parameter, we arrive at a purely electromagnetic action, but one in which the phase stiffness of the condensate L_ψ imparts a new quadratic term in the action of the electromagnetic field - a "mass term". Like a python that has swallowed its prey whole, the new gauge field is transformed into a much more sluggish object: it is heavy and weak. To see this in detail, let us re-examine Maxwell's in the presence of the mass term. Taking variations with respect to the fields, we obtain

$$\delta S_\psi = \int dtd^3x\,(\delta\mathbf{A}(x)\cdot\mathbf{j}(x) - \delta\varphi(x)\rho(x)) \tag{12.101}$$

where

$$\mathbf{j} = -\frac{1}{\mu_0\lambda_L^2}\mathbf{A}, \qquad \rho = -\frac{1}{\mu_0 c^{*2}\lambda_L^2}\varphi, \tag{12.102}$$

denote the superfluid velocity and the voltage-induced change in charge density, while

$$\delta S_{EM} = \frac{1}{\mu_0}\int dtd^3x\left[\delta\mathbf{A}\cdot\left(\frac{1}{c^2}\dot{\mathbf{E}} - \nabla\times\mathbf{B}\right) + \delta\varphi\frac{1}{c^2}\nabla\cdot\mathbf{E}\right]. \tag{12.103}$$

Setting $\delta S = \delta S_\psi + \delta S_{EM} = 0$, the vanishing of the coefficient of $\delta\varphi$ gives Gauss' equation

$$\frac{\delta S}{\delta\varphi} = \epsilon_0\nabla\cdot\mathbf{E} - \rho = 0, \tag{12.104}$$

while the vanishing of the coefficient of $\delta\mathbf{A}$ gives us Amperes equation,

$$\frac{\delta S}{\delta\mathbf{A}} = \frac{1}{\mu_0}\left(\frac{1}{c^2}\dot{\mathbf{E}} - \nabla\times\mathbf{B}\right) + \mathbf{j} = 0. \tag{12.105}$$

Since $\nabla\cdot(\nabla\times\mathbf{B}) = 0$, taking the divergence of (12.105) and using (12.104) to replace $\nabla\cdot\mathbf{E} = \rho/\epsilon$, leads to a continuity equation for the supercurrent

$$\nabla\cdot\mathbf{j} + \frac{\partial\rho}{\partial t} = -\frac{1}{\mu_0\lambda_L^2}\left(\nabla\cdot\mathbf{A} + \frac{1}{c^{*2}}\frac{\partial\varphi}{\partial t}\right) = 0, \tag{12.106}$$

excepting now, continuity also implies a gauge condition that ties ϕ to the longitudinal part of $\mathbf{A}$. For the relativistic case ($c^* = c$) this is the well-known Lorentz gauge condition ($\nabla_\mu A^\mu = 0$).

If we now expand Amperes equations in terms of $\mathbf{A}$, we obtain

$$\nabla\times\mathbf{B} = \nabla(\nabla\cdot\mathbf{A}) - \nabla^2\mathbf{A} = -\frac{1}{\lambda_L^2}\mathbf{A} + \frac{1}{c^2}\frac{\partial}{\partial t}\left(-\frac{\partial\mathbf{A}}{\partial t} - \nabla\varphi\right), \tag{12.107}$$

and using the continuity (12.106) to eliminate the potential term, we obtain

$$\left[\Box^2 - \frac{1}{\lambda_L^2}\right]\mathbf{A} = \left[1 - \left(\frac{c^*}{c}\right)^2\right]\nabla(\nabla\cdot\mathbf{A}), \tag{12.108}$$

where $\Box^2 = \nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}$. In a superconductor, where $c^* \neq c$, the right-hand side of (12.108) becomes active for longitudinal modes, where $\nabla\cdot\mathbf{A} \neq 0$. If we substitute $\mathbf{A} = A_o e^{i(\mathbf{p}\cdot\mathbf{x} - E_\mathbf{p} t)/\hbar}\hat{\mathbf{e}}$ into (12.108) we find that the dispersion $E(\mathbf{p})$ of the transverse and longitudinal photons are given by

$$E(\mathbf{p}) = \begin{cases} [(m_A c^2)^2 + (pc^*)^2]^{1/2}, & (\hat{\mathbf{e}} \perp \mathbf{p} \quad \text{longitudinal}) \\ [(m_A c^2)^2 + (pc)^2]^{1/2}, & (\hat{\mathbf{e}} \parallel \mathbf{p} \quad \text{transverse}) \end{cases} \tag{12.109}$$

Remarks:

- Both photons share the same mass gap but they have widely differing velocities[18, 20]. The slower longitudinal mode of the electromagnetic field couples to density fluctuations: this is the mode associated with the exclusion of electric fields from within the superconductor, and it continues to survive in the normal metal above T_c as a consequence of electric screening.

- The rapidly moving transverse mode, which couples to currents: this is the new excitation of the superconductor that gives rise to the Meissner screening of magnetic fields.

- For a relativistic case, the right-hand side of (12.108) vanishes and the longitudinal and transverse photons merge into a single massive photon[19], described by a "Klein Gordon" equation

$$\left[\Box^2 - \left(\frac{m_A c}{\hbar}\right)^2\right]\mathbf{A} = 0 \tag{12.110}$$

for a vector field of mass $m_A = \hbar/(\lambda_L c)$. The generation of a finite mass in a gauge field through the absorption of the phase degrees of freedom of an order parameter into a gauge field is the essence of the Anderson Higg's mechanism.

12.6.3 Electroweak theory

The standard model for electroweak theory, developed by Glashow, Weinberg and Salam[21, 22, 2] provides a beautiful example of how the idea of broken symmetry, developed for physics in the laboratory, also provides insight into physics of the cosmos itself. This is not abstract physics, for the sunshine we feel on our face is driven by the fusion of protons inside the sun. The rate limiting process is the conversion of two protons to a deuteron according to the reaction

$$p + p \to (pn) + e^+ + \nu_e$$

where the ν_e is a neutrino. This process occurs very slowly, due to the Coulomb repulsion between protons, and the weakness of the weak decay process that converts a proton into a neutron. Were it not for the weakness of the weak force, fusion would burn too rapidly, and the sun would have burnt out long before life could have formed on our planet. It is remarkable that the physics that makes this possible, is the very same physics that gives rise to the levitation of superconductors.

Electroweak theory posits that the electromagnetic and weak force derive from a common unified origin, in which part of the field is screened out of our universe through the development of a broken symmetry, associated with two component complex order parameter or "Higg's field"

$$\Psi = \begin{pmatrix}\psi_0\\ \psi_1\end{pmatrix}$$

that condenses in the early universe. The coupling of its phase gradients to gauge degrees of freedom generates the massive vector bosons of the weak nuclear force via the Anderson-Higg's effect, miraculously leaving behind one decoupled gapless mode that is the photon. Fluctuations in the amplitude of the Higg's condensate are predicted to give rise to a massive Higg's particle.

The basic physics of the standard model can be derived using the techniques of Ginzburg Landau theory, by examining the interaction of the Higg's condensate with gauge fields. In its simplest version, first written down by Weinberg [2], this is given by (see example 13.9)

$$S_\Psi = -\int d^4x \left[\frac{1}{2}|\left(\nabla_\mu - i\mathcal{A}_\mu\right)\Psi|^2 + \frac{u}{2}\left(\Psi^\dagger\Psi - 1\right)^2\right], \tag{12.111}$$

where relativistic notation $|\nabla_\mu\Psi|^2 \equiv |\nabla\Psi|^2 - |\dot{\Psi}|^2$ is used in the gradient term. The gauge field $\mathcal{A}_\mu$ acting on a two component order parameter is a two dimensional matrix made up of a U(1) gauge field B_a that couples to the charge of the Higg's field and an SU (2) gauge field $\vec{A}_\mu$,

$$\mathcal{A}_\mu = g\vec{A}_\mu \cdot \vec{\tau} + g' B_\mu$$

where $\vec{\tau}$ are the Pauli matrices and $\vec{A}_\mu = (A^1_\mu, A^2_\mu, A^3_\mu)$ is a triplet of three gauge fields that couple to the isospin of the condensate. When the Anderson Higg's effect is taken into account, three components of the Gauge fields acquire a mass, giving rise to two charged $W^\pm$ with mass M_W and one neutral Z boson of mass M_Z that couples to neutral currents of leptons and quarks.

$$\mathcal{A}_\mu \to \begin{cases} Z,\ W^\pm & \text{neutral/charged vector bosons} \\ A & \text{photon} \end{cases}$$

When S_Ψ is split up into amplitude and phase modes of the order parameter, it divides up into two parts (see example below) $S = S_H + S_W$, where

$$S_H = -\frac{1}{2}\int d^4x \left[(\nabla_\mu\phi_H)^2 + m_H^2\phi_H^2\right] \tag{12.112}$$

describes the amplitude fluctuations of the order parameter associated with the Higg's boson, where $m_H^2 = 4u$ defines its mass, while

$$S_W = -\frac{1}{2}\int d^4x \left[M_W^2(W^\dagger{}_\mu W^\mu) + M_Z^2(Z_\mu Z^\mu)\right] \tag{12.113}$$

determines the masses of the vector bosons.

The ratio of masses determines the weak-mixing angle θ_W

$$\cos(\theta_W) = \frac{M_W}{M_Z}$$

Experimentally, $M_Z = 91.19$ GeV/c^2 and $M_W = 80.40$ GeV/c^2, corresponding to a Weinberg angle of $\theta_W \approx 28^0$. The Higg's particle has not yet been observed, and estimates of its mass vary widely, from values as low as 80GeV/c^2, to values an order of magnitude higher.

From the perspective of superconductivity, these two numbers define two length scales: a "penetration depth" for the screened weak fields of order

$$\lambda_W = \frac{\hbar}{m_W c} \sim 2\times 10^{-18}\text{m}$$

which defines the range of the weak force. At present, the "coherence length" of electroweak theory. If one uses the estimated Higg's mass, this is a length of order[23]

$$\xi_W = \frac{\hbar}{m_H c} \sim 2\times 10^{-18} - 2\times 10^{-19}\text{m}.$$

This very wide range of scales leaves open the possibility that the condensed Higg's field is either weakly type *I*, or strongly type *II* in character, an issue of importance to theories of the early universe. The microscopic physics that develops below the coherence length ξ_W is also an open mystery that is the subject of ongoing measurements at the Large Hadron Collider.

Table II contrasts the physics of superconductivity with the electroweak physics.

	Superconductivity	Electro-weak
Order parameter	ψ Pair condensate	$\begin{pmatrix}\psi_0\\ \psi_1\end{pmatrix}$ Higg's condensate
Gauge field/Symmetry	$(\phi, \mathbf{A})$ U (1)	$\mathcal{A}_\mu = g' B_\mu + g(\vec{A}_\mu \cdot \vec{\tau})$ U (1)×SU(2)
Penetration depth	$\lambda_L \sim 10^{-7}$m	$\lambda_W \sim 10^{-18}$m
Coherence length	$\xi = \frac{v_F}{\Delta} \sim 10^{-9} - 10^{-7}$m	$\xi_{EW} \sim 10^{-18} - 10^{-19}$m
Condensation mechanism	pairing	unknown
Screened field	$\vec{B}$	$W^\pm$, Z
Massless gauge field	None	Electromagnetism A_μ

Example 12.10:

(a) Suppose the Higg's condensate is written $\Psi(x) = (1 + \phi_H(x))U(x)\Psi_0$, where ϕ_H is a real field, describing small amplitude fluctuations of the condensate, $U(x)$ is a matrix describing the slow variations in orientation of the order parameter and $\Psi_0 = \begin{pmatrix}1\\0\end{pmatrix}$ is just a unit spinor. Show that the the action splits into two terms, $S = S_H + S_W$, where

$$S_H = -\frac{1}{2}\int d^4x \left[(\nabla_\mu \phi_H)^2 + m_H^2 \phi_H^2\right] \tag{12.114}$$

describes the amplitude fluctuations of the order parameter associated with the Higg's boson, where $m_H^2 = 4u$ defines its mass, while

$$S_W = -\frac{1}{2}\int d^4x |\mathcal{A}'_\mu \Psi_0|^2. \tag{12.115}$$

determines the masses of the vector bosons.

(b) By expanding out the quadratic term in (12.115), show that it is diagonalized in terms of two gauge fields

$$S_W = -\frac{1}{2}\int d^4x \left[M_W^2 (W^\dagger{}_\mu W^\mu) + M_Z^2 (Z_\mu Z^\mu)\right]$$

and give the form of the fields and their corresponding masses in terms of the original fields and coupling constants.

Solution:

(a) Let us substitute

$$\Psi(x) = (1 + \phi_H(x))U(x)\Psi_0$$

where $\Psi_0 = \begin{pmatrix}1\\0\end{pmatrix}$, into (12.111) Since $\Psi^\dagger\Psi = (1+\phi_H)^2 \Psi_0{}^\dagger U^\dagger U \Psi_0 = (1+\phi_H)^2$, so to quadratic order, the "potential" part of S_Ψ can be written as

$$\frac{u}{2}(\Psi^\dagger\Psi - 1)^2 = \frac{u}{2}(2\phi_H + \phi_H^2)^2 = \frac{m_H}{2}\phi_H^2 + O(\phi_H^3). \qquad (m_H^2 = 4u)$$

The derivatives in the gradient term can be expanded as

$$(\nabla_\mu - i\mathcal{A}_\mu)\Psi(x) = (\nabla_\mu - i\mathcal{A}_\mu)U\Psi_0 + \nabla_\mu \phi_H (U\Psi_0).$$

Since the derivative of a unit spinor is orthogonal to itself, the two terms in the above expression are orthogonal so that when we take the modulus squared of the above expression, we obtain

$$\begin{aligned} |(\nabla_\mu - i\mathcal{A}_\mu)\Psi|^2 &= |(\nabla_\mu - i\mathcal{A}_\mu)U\Psi_0|^2 + (\nabla_\mu\phi_H)^2 \overbrace{|U\Psi_0|^2}^{=|\Psi_0|^2=1} \\ &= |U^\dagger(A_\mu + i\nabla_\mu)U\Psi_0|^2 + (\nabla_\mu\phi_H)^2 \end{aligned} \tag{12.116}$$

Here, we have introduced a pre-factor $iU^\dagger$ into the first term, which does not change its magnitude. Now the combination

$$\mathcal{A}'_\mu = U^\dagger(\mathcal{A}_\mu + i\nabla_\mu)U$$

is a gauge transformation of A_μ which leaves the physical fields ($G_{\mu\nu} = \nabla_\mu \mathcal{A}_\nu - \nabla_\nu \mathcal{A}_\mu - i[\mathcal{A}_\mu, \mathcal{A}_\nu]$) and the action associated with the gauge fields invariant. In terms of this transformed field, the gradient terms of S_Ψ can be written simply as

$$|(\nabla_\mu - i\mathcal{A}_\mu)\Psi|^2 = |\mathcal{A}'_\mu \Psi_0|^2 + (\nabla_\mu\phi_H)^2.$$

so that the sum of the gradient and potential terms yields

$$\begin{aligned} L &= -\frac{1}{2}|\left(\nabla_\mu - i\mathcal{A}_\mu\right)\Psi|^2 + \frac{u}{2}\left(\Psi^\dagger\Psi - 1\right)^2 \\ &= \overbrace{-\frac{1}{2}|\mathcal{A}'_\mu\Psi_0|^2}^{L_W} \underbrace{-\frac{1}{2}\left[(\nabla_\mu\phi_H)^2 + m_H^2\phi_H^2\right]}_{L_H} \end{aligned} \tag{12.117}$$

which when integrated over space-time, gives the results (SH) and (vbosons).

(b) Written out explicitly, the gradient appearing in the gauge theory mass term is

$$\begin{aligned}\mathcal{A}'_\mu\Psi_0 &= \left[g'B_\mu + g\vec{A}_\mu\cdot\vec{\tau}\right]\cdot\Psi_0 \\ &= \left[g'\begin{pmatrix}B_\mu & \\ & B_\mu\end{pmatrix} + g\begin{pmatrix}A^3_\mu & A^1_\mu - iA^2_\mu \\ A^1_\mu + iA^2_\mu & -A^3_\mu\end{pmatrix}\right]\begin{pmatrix}1\\0\end{pmatrix} \\ &= \begin{pmatrix}g'B_\mu + gA^3_\mu \\ g(A^1_\mu + iA^2_\mu)\end{pmatrix} \qquad (12.118)\end{aligned}$$

so that the mass term of the gauge fields can be written

$$\begin{aligned}L_W &= -\frac{1}{2}|\mathcal{A}_\mu\Psi|^2 = -\frac{1}{2}\left[(gA^3_\mu + g'B_\mu)^2 + g^2|A^1_\mu + iA^2_\mu|^2\right] \\ &= -\frac{M_Z^2}{2}Z_\mu^2 - \frac{M_W^2}{2}|W_\mu|^2 \qquad (12.119)\end{aligned}$$

where

$$\begin{aligned}W_\mu &= A^1_\mu + iA^2_\mu, \\ Z_\mu &= \frac{1}{\sqrt{g^2+(g')^2}}\left(g'A^{(3)}_\mu + gB_\mu\right) \qquad (12.120)\end{aligned}$$

are respectively, the charged W and neutral Z bosons which mediate the weak force, $M_Z = \sqrt{g^2+g'^2}$ and $M_W = g = M_Z cos[\theta_W]$, where θ_W is the Weinberg angle determined by

$$\cos\theta_W = \frac{g}{\sqrt{g^2+g'^2}}.$$

12.7 The concept of generalized rigidity

The "phase rigidity" responsible for superflow, the Meissner effect and its electro-weak counterpart, are each consequences of general property of broken continuous symmetries. In any broken continuous symmetry, the order parameter can assume any one of continouous number of directions, each with precisely the same energy. By contrast, it always costs an energy to slowly "bend" the direction of the order-parameter away from a state of uniform order. This property is termed "generalized rigidity" [24]. In a superconductor or superfluid, it costs a phase bending energy

$$U(x) \sim \frac{1}{2}\rho_s(\nabla\phi(x))^2, \qquad (12.121)$$

to create a gradient of the phase. The differential of U with respect to the phase gradient $\delta U/(\hbar\delta\nabla\phi)$ defines the "superflow" of particles is directly proportional to the amount of phase bending, or the gradient of the phase

$$j_S = \frac{\delta U}{\hbar\delta\nabla\phi} = \frac{\rho_s}{\hbar}\nabla\phi. \qquad (12.122)$$

This relationship holds because density and phase are conjugate variables. Anderson noted that that we can generalize this concept, to a wide variety of broken symmetries, each with their corresponding phase and conjugate conserved quantity. In each case, a gradient of the order parameter gives rise to a "superflow" of the quantity that translates the phase(see table 1).

For example, broken translation symmetry leads to the superflow of momentum, or sheer stress, broken spin symmetry leads to the superflow of spin or spin superflow. There are undoubtedly new classes of broken symmetry yet to be discovered - one of which might be broken time translational invariance (see table 1).

Table. 1. Order parameters, broken symmetry and rigidity.

Name	Broken Symmetry	Rigidity/Supercurrent
Crystal	Translation Symmetry	Momentum superflow (Sheer stress)
Superfluid	Gauge symmetry	Matter superflow
Superconductivity	E.M. Gauge symmetry	Charge superflow
Antiferromagnetism	Spin rotation symmetry	Spin superflow (x-y magnets only)
?	Time Translation Symmetry	Energy superflow ?

12.8 Thermal Fluctuations and criticality

At temperatures that are far below, or far above a critical point, the behavior of the order parameter resembles a tranquil ocean with no significant amount of thermal noise in its fluctuations. But fluctuations become increasingly important near the critical point as the correlation length diverges. At the second-order phase transition, infinitely long-range **"critical fluctuations"** develop in the order parameter. The study of these fluctuations requires that we go beyond mean field theory. Instead of using the Landau Ginzburg functional as a variational Free energy, now we use it to determine the Boltzmann probability distribution of the thermallly fluctuating order parameter, as follows

$$p[\psi] = Z^{-1}e^{-\beta F_{GL}[\psi]} = \frac{1}{Z}\exp\left[-\beta\int d^dx\left(\frac{1}{2}\left[s(\nabla\psi)^2 + r|\psi(x)|^2\right] + u|\psi(x)|^4\right)\right]$$

where $Z = \sum_\psi e^{-\beta F_{GL}[\psi]}$ is the normalizing partition function. This is the famous "ϕ^4 field theory" of statistical mechanics (where we use ψ in place of ϕ.)

The variational approach can be derived from the probability distribution function $p[\{\psi\}]$, by observing that the probabilitly of a given configuration is sharply peaked around around the mean field solution, $\psi = \psi_0$. If we make a Taylor expansion around around a nominal mean-field configuration, writing $\psi(x) = \psi_0 + \delta\psi(x)$, then

$$F_{GL}[\{\psi\}] = F_{mf} + \int_x \delta\psi(x) \overbrace{\frac{\delta F_{GL}}{\delta\psi(x)}}^{=0} + \frac{1}{2}\int_{x,x'} \delta\psi(x)\delta\psi(x')\frac{\delta^2 F_{GL}}{\delta\psi(x)\delta\psi(x')} + \ldots$$

where the first derivative is zero because the Free energy is stationary for the mean-field solution $\delta F/\delta\psi = 0$, which implies

$$F_{GL}[\{\psi\}] = F_{mf}[\psi_0] + \frac{1}{2}\int_{x,x'} \delta\psi(x)\delta\psi(x')\frac{\delta^2 F_{GL}}{\delta\psi(x)\delta\psi(x')} + \ldots$$

The first non-vanishing terms in the Free energy are second order terms, describing a Gaussian distribution of the fluctuations of the order parameter about its average

$$\delta\psi(x) = \psi(x) - \psi_0$$

The amplitude of the fluctuations at long wavelengths becomes particularly intense near a critical point. This point was first appreciated by Ornstein and Zernicke, who observed in 1914 that light scatters strongly off the long-wavelength density fluctuations of a gas near the critical point of the liquid-gas phase transition. We now follow Ornstein Zernicke's original treatment, and study study the behavior of order parameter fluctuations above the phase transition.

To treat the fluctuations we Fourier transform the order parameter:

$$\psi(x) = \frac{1}{\sqrt{V}}\sum_{\mathbf{q}} \psi_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}}, \qquad \psi_{\mathbf{q}} = \frac{1}{\sqrt{V}}\int d^d x \psi(x) e^{-i\mathbf{q}\cdot\mathbf{x}}. \tag{12.123}$$

Here, we use periodic boundary conditions in a finite box of volume $V = L^d$, with discrete wavevectors $\mathbf{q} = \frac{2\pi}{L}(l_1, l_2, \ldots l_d)$. Note that $\psi_{-\mathbf{q}} = \psi^*_{\mathbf{q}}$, since ψ (or each of its $n-$ components) is real. Substituting 12.123 into 12.15, noting that $(-s\nabla^2 + r) \to (sq^2 + r)$ inside the Fourier transform, we obtain

$$F = \frac{1}{2}\sum_{\mathbf{q}} |\psi_{\mathbf{q}}|^2 \left(sq^2 + r\right) + u\int d^d x |\psi(x)|^4. \tag{12.124}$$

so that the quadratic term is diagonal in the momentum-space representation. Notice how we can rewrite the GL energy in terms of the (bare) susceptibility $\chi_{\mathbf{q}} = (sq^2 + r)^{-1}$ encountered in (12.19), as

$$F = \frac{1}{2}\sum_{\mathbf{q}} |\psi_{\mathbf{q}}|^2 \chi^{-1}_{\mathbf{q}} + u\int d^d x |\psi(x)|^4. \tag{12.125}$$

so the quadratic coefficient of the GL free energy is the inverse susceptibilty.

Suppose $r > 0$ and the deviations from equilibrium $\psi = 0$ are small enough to ignore the interaction, permitting us to temporarily set $u = 0$. In this case, F is a simple quadratic function of $)\psi_{\mathbf{q}}$ and the probability distribution function is a simple Gaussian

$$p[\psi] = Z^{-1}\exp\left[-\frac{\beta}{2}\sum_{\mathbf{q}} |\psi_{\mathbf{q}}|^2\left(sq^2 + r\right)\right] \equiv Z^{-1}\exp\left[-\sum_{\mathbf{q}}\frac{|\psi_{\mathbf{q}}|^2}{2S_{\mathbf{q}}}\right]$$

where

$$S_{\mathbf{q}} = \langle|\psi_{\mathbf{q}}|^2\rangle = \frac{k_B T}{sq^2 + r} = \frac{k_B T/c}{q^2 + \xi^{-2}}. \tag{12.126}$$

is the variance of the fluctuations at wavevector $\mathbf{q}$ and $\xi = \sqrt{s/r}$ is the correlation length. This distribution function is known as the "Ornstein-Zernicke" form for the Gaussian variance of the order parameter. This quantity is the direct analog of the Green's function in many body physics. Note that

- For $q >> \xi^{-1}$, $S_q \propto 1/q^2$ is singular or "critical".
- Using (12.19) we see that the fluctuations of the order parameter are directly related to its static susceptibility. $S_{\mathbf{q}} = k_B T\chi_{\mathbf{q}}$. This is a consequence of the fluctuation dissipation theorem in the classical limit.
- S_q resembles a Yukawa interaction associated with the virtual exchange of massive particles : $V(q) = 1/(q^2 + m^2)$. Indeed, short-range nuclear interactions are a result of quantum fluctuations in a pion field with correlation length $\xi \sim m^{-1}$.

Next, let us Fourier transform this result to calculate the spatial correlations:

$$\begin{aligned} S(\mathbf{x} - \mathbf{x}') = \langle\delta\psi(x)\delta\psi(x')\rangle &= \frac{1}{V}\sum_{\mathbf{q},\mathbf{q}'} \overbrace{\langle\psi_{-\mathbf{q}}\psi_{\mathbf{q}'}\rangle}^{S_{\mathbf{q}}\delta_{\mathbf{q}-\mathbf{q}'}} e^{i(\mathbf{q}'\cdot\mathbf{x}' - \mathbf{q}\cdot\mathbf{x})} \\ &= \int \frac{d^d q}{(2\pi)^d}\frac{k_B T/c}{q^2 + \xi^{-2}} e^{i\mathbf{q}\cdot(\mathbf{x}'-\mathbf{x})} \end{aligned} \tag{12.127}$$

where we have taken the thermodynamic limit $V \to \infty$. This is a Fourier transform that we have encountered in conjunction with the screened Coulomb interaction, and in three dimensions we obtain

$$S(\mathbf{x} - \mathbf{x}') = \frac{k_B T}{4\pi s}\frac{e^{-|\mathbf{x}-\mathbf{x}'|/\xi}}{|\mathbf{x} - \mathbf{x}'|}, \qquad (d = 3)$$

Note that:

- The generalization of this result to d dimensions gives

$$S(\mathbf{x}) \sim \frac{e^{-x/\xi}}{x^{d-2+\eta}}$$

where Ginzburg Landau theory predicts $\eta = 0$.

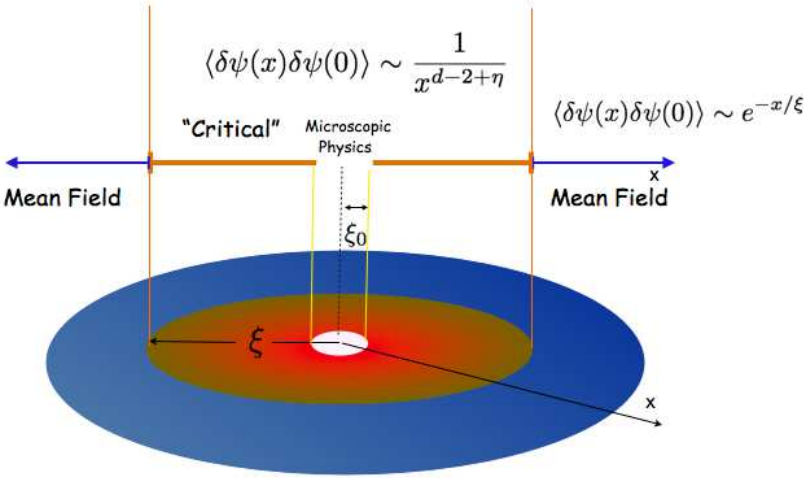

Figure 12.11: Length-scales near a critical point. On length-scales $\xi >> x >> \xi_0$, fluctuations are critical, with universal power-law correlations. On length-scales larger than the correlation length ξ, fluctuations are exponentially correlated. On length scales shorter than the coherence length ξ_0, the order parameter description must be replaced by a microscopic description of the physics.

- $S(\mathbf{x})$ illustrates a very general property. On length scales below the correlation length, the fluctuations are critical, with power-law correlations, but on longer length scales, correlations are exponentially suppressed. (See Fig. 12.11).
- Ginzburg Landau theory predicts that the correlation length diverges as

$$\xi \propto (T - T_c)^{-\nu}$$

where $\nu = 1/2$. Remarkably, even though Ginzburg Landau theory neglects the non-linear interactions of critical modes, these results are qualitatively correct. More precise treatments of critical phenomenon show that the exponents depart from Gaussian theory in dimensions $d < 4$.

12.8.1 Limits of mean-field Theory: Ginzburg Criterion

What are the limits of mean-field theory? We studied the fluctuations at temperatures $T > T_c$ by assuming that the non-linear interaction term can be ignored. This is only true provided the amplitude of fluctuations is sufficiently small. The precise formulation of this criterion was first proposed by Levanyuk[25] and Ginzburg[26]. The key observation here, is that mean-field theory is only affected by fluctuations on length-scales longer than the correlation length $x >> \xi$. Fluctuations on wavelengths shorter than the correlation length are absorbed into renormalized Landau parameters and do not produce departures from mean-field theory. To filter out the irrelevant short-wavelength fluctuations, we need to consider a coarse-grained average $\bar{\psi}$ of the order parameter over a correlation volume ξ^d. The Ginzburg criterion simply states that variance of the averaged order parameter must be small compared with the equilibrium value, i.e

$$\delta\bar{\psi}^2 = \frac{1}{\xi^d}\int_{|x|<\xi} d^d x \langle \delta\psi(x)\delta\psi(0)\rangle << \psi_0^2 \tag{12.128}$$

Since correlations decay exponentially on length-scales longer than ξ, to get an an estimate of this average, we can remove the constraint $|x| < \xi$ on the volume integral, to obtain

$$\delta\bar{\psi}^2 \sim \frac{1}{\xi^d}\int d^d x \langle \delta\psi(x)\delta\psi(0)\rangle \sim \frac{S_{\mathbf{q}=0}}{\xi^d} = \frac{k_B T_c}{s\,\xi^{d-2}}$$

Now substituting $\psi_0^2 = \frac{|r|}{4u} \sim \frac{s}{u}\frac{1}{\xi^2}$ we obtain

$$\frac{\delta\bar{\psi}^2}{\psi_0^2} \sim \frac{k_B T_c}{\xi^{d-4}}\frac{u}{s^2} << 1.$$

or

$$\xi^{4-d} << \frac{c^2}{k_B T_c}.$$

Let us try to understand the meaning of the length-scale defined by this expression. Multiplying by this expression by ξ_0^{d-4}, where $\xi_0 = \sqrt{s/(aT_c)}$ is the coherence length, we obtain the dimensionless criterion

$$\left(\frac{\xi}{\xi_0}\right)^{4-d} << \xi_0^d \frac{\overbrace{s^2\xi_0^{-4}}^{(aT_c)^2}}{uk_B T_c} = \xi^d \frac{a^2 T_c}{uk_B}$$

Now from (12.11) we recognize the combination $\frac{a^2 T_c}{u} = 8\Delta C_V$ as the jump in the specific heat, so that the Ginzburg criterion can be written in the form

$$\boxed{\left(\frac{\xi}{\xi_0}\right)^{4-d} << \frac{S_G}{k_B}, \qquad S_G = \Delta C_V \xi_0^d \qquad \text{Ginzburg Criterion,}} \tag{12.129}$$

where we have dropped the factor of 8. The quantity $S_G = \Delta C_V \xi_0^d$, has the dimensions of entropy, and can be loosely interpreted as the entropy reduction per coherence volume ξ_0^d associated with the development of order, so that $S_G/k_B = \ln W$ is a logarithmic measure number of degrees of freedom W associated with the fully-developed order parameter.

For models with $d > 4$, the Ginzburg criterion implies that large correlation lengths are good and in this situation, as the correlation length diverges close to the critical point, mean-field theory becomes essentially exact. The dimension $d_U = 4$ is called the upper critical dimension. In a realistic situation, where $d < d_U = 4$ $d < 4$, ξ^{4-d} diverges as the critical point is approached, so for $d < d_U = 4$, the Ginzburg criterion sets an upper bound on the correlation length and lower bound on the distance from the phase transition. If we rewrite $\xi/\xi_0 = |\Delta T/T_c|^{-1/2}$, the temperature deviation from T_c, ΔT must satisfy the requirement

$$\frac{|\Delta T|}{T_c} >> (S_G/k_B)^{-(4-d)2} \tag{12.130}$$

for mean-field theory to be reliable.

From the above discussion, it is clear that systems with a large coherence length will deviate from mean-field theory only over a very narrow temperature window. Examples of systems with large coherence lengths are superconductors, superfluid $He-3$ and spin density waves, where the ratio between the transition temperature and the Fermi temperature of the fluid $k_BT_c/\epsilon_F << 1$. For example, in a superconductor, the entropy of fondensation per unit cell is of order $k_B(\epsilon/\Delta)$, where $\Delta \sim 3.5k_BT_c$ is the gap, while the coherence length is of order $v_F/\Delta \sim a(\epsilon_F/\Delta)$, where $v_F \sim \epsilon_F a$ is the Fermi velocity, so that the entropy of condensation per coherence length is of order

$$\Delta S_G/k_B \sim (\Delta/\epsilon_F) \times (\epsilon_F/\Delta)^3 \sim (\epsilon_F/\Delta)^2$$

and the Ginburg criterion is

$$\frac{|\Delta T|}{T_c} >> (\Delta/\epsilon_F)^4$$

in three dimensions. Similar arguments may be applied to charge and spin density wave materials. For a typical superconductor with $T_c \sim 10K$, $\Delta \sim 30K$, $\epsilon_F \sim 10^5 K$, this gives $\frac{|\Delta T|}{T_c} \sim (10^{-5})^4 \sim 10^{-20}$, far beyond the realm of observation. By contrast, in an insulating magnet the coherence length is of order the lattice spacing, a and the "Ginzburg entropy" is of order unity so $\Delta T/T_c \sim 1$. These discussions are in accord with observations. Superconductors and charge density wave systems display perfect mean-field transitions, yet insulating magnets and superfluid $He-3$ display the classic λ-shaped specific heat curves that are a hall-mark of a non-trivial specific-heat exponent α.

12.9 Exercises

1. Show that the action of $U(\phi)e^{i\phi\hat{N}}$ on a coherent state, $|\phi\rangle = U^\dagger(\phi)|\psi\rangle$ uniformly shifts the phase of the order parameter by ϕ, i.e.

   $$\hat{\psi}(x)|\phi\rangle = \psi(x)e^{i\phi}|\phi\rangle$$

   so that

   $$-i\frac{d}{d\phi}|\phi\rangle = \hat{N}|\phi\rangle$$

Solution:

(a) Let us begin by showing that $U(\phi)\hat{\psi}^\dagger(x)U^\dagger(\phi) = e^{i\phi}\hat{\psi}^\dagger(x)$. Since $\hat{\psi}^\dagger$ adds a particle to a state, it follows that

$$\hat{\psi}^\dagger(x)|\alpha, N\rangle = |\beta, N+1\rangle.$$

where $|\alpha, N\rangle$ and $|\beta, N+1\rangle$ are states with N and $N+1$ particles, respectively. But then

$$e^{i\phi\hat{N}}\hat{\psi}^\dagger(x)\overbrace{e^{-i\phi\hat{N}}|\alpha, N\rangle}^{e^{-i\phi N}|\beta,N+1\rangle} = e^{i\phi(N+1)}\hat{\psi}^\dagger(x)e^{-i\phi N}|\alpha, N\rangle = e^{i\phi}\hat{\psi}^\dagger(x)|\alpha, N\rangle$$

Since this holds for all states $|\alpha, N\rangle$, it follows that

$$U(\phi)\hat{\psi}^\dagger(x)U^\dagger(\phi) = e^{i\phi}\hat{\psi}^\dagger(x)$$

(b) Let us write out $|\phi\rangle = U(\phi)|\psi\rangle$ explicitly:

$$U(\phi)|\psi\rangle = U(\phi)\exp\left[\int d^dx\psi(x)\hat{\psi}^\dagger(x)\right]U^\dagger(\phi)|0\rangle$$

where we have sneaked in a $U^\dagger(\phi)$ just before the vacuum, since $U^\dagger(\phi)|0\rangle = |0\rangle$. Using the identity $Ue^AU^\dagger = e^{UAU^\dagger}$, we can move the unitary operators inside the exponential

$$\begin{aligned} U(\phi)|\psi\rangle &= \exp\left[\int d^dx\psi(x)\overbrace{U(\phi)\hat{\psi}^\dagger(x)U^\dagger(\phi)}^{e^{i\phi}\hat{\psi}^\dagger(x)}\right]|0\rangle \\ &= \exp\left[\int d^dx(\psi(x)e^{i\phi})\hat{\psi}^\dagger(x)\right]|0\rangle \end{aligned} \tag{12.131}$$

corresponding to a coherent state where $\psi(x) \to \psi(x)e^{i\phi}$ has picked up an additional uniform phase.

(c) Since $|\phi\rangle = e^{i\phi\hat{N}}|\psi\rangle$, differentiating both sides with respect to ϕ, we obtain

$$-i\frac{d}{d\phi}|\phi\rangle = -i\overbrace{\frac{d}{d\phi}\left[e^{i\phi\hat{N}}\right]}^{i\hat{N}e^{i\phi\hat{N}}}|\psi\rangle = \hat{N}|\phi\rangle.$$

Since this holds for all such coherent states, it follows that $\hat{N} = -i\frac{d}{d\phi}$.

2. Consider the most general form of a two component Landau theory

$$f[\psi] = \frac{r}{2}(\psi_1^2 + \psi_2^2) + \frac{s}{2}(\psi_1^2 - \psi_2^2) + u(\psi_1^2 + \psi_2^2)^2 + u_2(\psi_1^4 - \psi_2^4) + u_3\psi_1^2\psi_2^2$$

   (a) Rewrite the free energy in terms of the amplitude and phase of the order parameter to demonstrating that if s, u_2 or u_3 are finite, the free energy is no longer gauge invariant.

   (b) Rewrite the free energy as a function of ψ and ψ^*.

   (c) If $s > 0$, what symmmetry is broken when $r < 0$?

   (d) Write down the mean field equations for $s = 0, r < 0$.

(e) Sketch the phase diagram in the (u_2, u_3) plane.

3. Consider the more general class of Landau theory where the interaction u can be negative:

$$f[\psi] = \frac{1}{V}F[\psi] = \frac{r}{2}\psi^2 + u_4\psi^4 + u_6\psi^6 - h\psi$$

(a) Show that for $h = 0, u < 0, r > 0$ the free energy contains three local minima, one at $\psi = 0$ and two others at $\psi = \pm\psi_0$, where

$$\psi_0^2 = -\frac{u}{3u_6} \pm \sqrt{\left(\frac{u}{3u_6}\right)^2 - \frac{r}{6u_6}}.$$

(b) Show that for $r < r_c$, the solution at $\psi = 0$ becomes metastable, giving rise to a first order phase transition at

$$r_c = -\frac{u^2}{2u_6}$$

(Hint: Calculate the critical value of r by imposing the second condition $f[\psi_{II}] = 0$. Solve the equation $f[\psi] = 0$ simultaneously with $f'[\psi_0] = 0$ from the last part.)

(c) Sketch the (T, u) phase diagram for $h = 0$.

(d) For $r = 0$ but $h \neq 0$ show that there are three lines of critical points where $f'[\psi] = f''[\psi] = 0$ converging at the single point $r = u = h = 0$. This point is said to be a "tricritical point".

(e) Sketch the (h, u) phase diagram for $r = 0$.

4. We can construct a state of bosons in which the bosonic field operator has a definite expectation value using a coherent state as follows

$$|\psi\rangle = \exp\left[\int d^3x \psi\hat{\psi}^\dagger(x)\right]|0\rangle.$$

The Hermitian conjugate of this state is $\langle\bar{\psi}| = \langle 0|e^{\int d^3x\hat{\psi}(x)\psi^*}$.

(a) Show that this coherent state is an eigenstate of the field destruction operator: $\hat{\psi}(x)|\psi\rangle = \psi|\psi\rangle$.

(b) Show that overlap of the coherent state with itself is given by $\langle\bar{\psi}|\psi\rangle = e^N$, where $N = V|\psi|^2$ is the number of particles in the condensate.

(c) If

$$H = \int d^3x \left[\hat{\psi}^\dagger(x)\left(-\frac{\hbar^2}{2m}\nabla^2 - \mu\right)\psi(x) + U : (\psi^\dagger(x)\psi(x))^2 :\right]$$

is the (normal ordered) energy density, show that the energy density $f = \frac{1}{V}\langle H\rangle$, where

$$\langle H\rangle = \frac{\langle\bar{\psi}|H|\psi\rangle}{\langle\bar{\psi}|\psi\rangle}$$

is given by

$$f = -\mu|\psi|^2 + U|\psi|^4.$$

providing a direct realization of the Landau Free energy functional.

5. (Systematic derivation of the Ginzburg criterion).

(a) Show that the Ginzburg Landau free energy (12.125) can be written in the form

$$F = \frac{1}{2}\int d^dx' d^dx \psi(x')\chi_0^{-1}(x' - x)\psi(x') + u\int d^dx \psi(x)^4. \tag{12.132}$$

where

$$\chi_0^{-1}(x' - x) = \delta^d(x - x')\left[-s\nabla^2 + r\right]$$

is inverse of the susceptibility. The subscript "0" has been added to χ^{-1} denoting that is the "bare" susceptibilty, calculated for $u = 0$.

(b) By identifying the renormalized susceptibility with the second derivative of the free energy, show that when interactions are taken into account

$$\chi_0^{-1}(x' - x) \approx \langle\frac{\delta^2 F}{\delta\psi(x)\delta\psi(x')}\rangle = \delta^d(x' - x)\left[-s\nabla^2 + r + 12u\langle\psi^2\rangle\right]$$

(Hint: differentiate (12.17) with respect to $\psi(x)$ and take the expectation value of the resulting expression), so that in momentum space

$$\chi_{\mathbf{q}} = sq^2 + r + 12u\langle\psi^2\rangle_T$$

where $\langle\psi^2\rangle_T = S(\mathbf{x} - \mathbf{x}')|_{\mathbf{x}=\mathbf{x}'}$ is the variance of the order parameter at a single point in space, evaluated at temperature T.

(c) Show that the effects of fluctuations suppress T_c, and that at the new suppressed transition temperature T_c^*

$$r = r_0 = a(T_c^* - T_c) = -12u\langle\psi^2\rangle_{T_c^*} = -12u\int \frac{d^dq}{(2\pi)^d}\frac{k_BT_c^*/c}{q^2}.$$

so that

$$\chi_{\mathbf{q}}^{-1} = sq^2 + (r - r_0) + 12u\left[\langle\psi^2\rangle - \langle\psi^2\rangle_{T_c^*}\right]$$

Notice how the subtraction of the fluctuations at $T = T_c^*$ renormalizes $r \to r - r_0 = a(T - T_c^*)$. What is the renormalized correlation length?

(d) Finally, calculate the Ginzburg criterion by requiring that $|r - r_0| > 12u\left[\langle\psi^2\rangle - \langle\psi^2\rangle_{T_c^*}\right]$, to obtain

$$\frac{|r - r_0|}{4u} < 3\int \frac{d^dq}{(2\pi)^d}\frac{k_BT_c^*}{q^2}\left[\frac{\xi^{-2}}{q^2 + \xi^{-2}}\right] \tag{12.133}$$

The term inside the square brackets on the right hand side results from the renormalization of $r \to r - r_0$. Notice how this term only involves fluctuations with $q \leq \xi^-1$, i.e the long-wavelength fluctuations of wavelength greater than ξ. What has happened to the short wavelength fluctuations

(e) By approximately evaluating the integral on the right-hand side of (12.133) obtain the Ginzburg criterion:

$$\frac{|r - r_0|}{u} << \frac{k_BT_c^*}{s}\frac{1}{\xi^{d-2}}$$

6. Properties of a coherent state.

Show that a coherent state $|\alpha\rangle = e^{\alpha a^\dagger}|0\rangle$ can be expanded as a sum of Harmonic oscillator states $|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle$, as follows

$$|a\rangle = |0\rangle + a|1\rangle + \ldots \frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

(b) Show that $\langle \alpha^* | \alpha \rangle = e^{|\alpha|^2}$, so that a normalized coherent state is given by

$$|\alpha\rangle_N = e^{-|\alpha|^2/2} e^{\alpha \hat{a}^\dagger} |a\rangle$$

(c) Show that the probabilty of being in a state with n particles is a Poisson distribution

$$p(n) = \frac{(\lambda)^n}{n!} e^{-|\lambda|}, \qquad \lambda = |\alpha|^2$$

Note that a Poission distribution has equal mean and variance : $\langle \hat{N} \rangle = \langle \delta \hat{N}^2 \rangle = \lambda$

(d) Show that when $\alpha = \sqrt{N_s}$, $\frac{\delta N^2}{N^2} = \frac{1}{N_s}$.

(e) Show that when the superconducting order parameter is written in terms of its amplitude and phase, $\psi = |\psi| e^{i\phi}$, that the Ginzburg Landau free energy of a superconductor separates into a phase and an amplitude component.

$$\begin{aligned} \left| \left(\nabla - i \frac{q}{\hbar} \mathbf{A} \right) \psi \right|^2 &= \left| e^{i\phi} \left[\nabla |\psi| + i \left(\nabla \phi - \frac{q}{\hbar} \mathbf{A} \right) \right] \right|^2 \\ &= (\nabla |\psi|)^2 + |\psi|^2 \left(\nabla \phi - \frac{q}{\hbar} \mathbf{A} \right)^2 \end{aligned} \tag{12.134}$$

Use this expression to rederive an expression for the current in terms of the phase gradient of the order parameter.

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Chapter 13

Path Integrals

13.1 Broken symmetry, coherent states and path integrals.

In this chapter, we link the order parameter concept with microscopic Many Body Physics by introducing the path integral formulation of quantum many body theory. The emergence of a macroscopic order parameter in a quantum system is analogous to the emergence of classical mechanics in macroscopic quantum systems. The emergence of classical mechanics from quantum mechanics is most naturally described using wave-packets and the Feynman path integral. We shall see that a similar approach is useful for many body systems, where the many body "wave-packets" states are coherent states: eigenstates of the quantum fields.

Chapter 12 introduced Landau's concept of broken symmetry, embracing the idea of an order parameter $\Psi(x)$. The beauty of the Landau approach, is that it is a macroscopic description of matter: a length scales beyond the microscopic coherence length ξ_0, the emergence of an order parameter does not depend on the detailed microscopic microscopic physics that gives rise to it. In this chapter we go beneath the coherence length, to examine the connection between the order parameter and the microscopic physics of a many body system.

The basic idea of Feynman's path integral[1, 2, 3], is to re-formulate the quantum mechanical amplitude as sum of contributions from all possible paths, in which the classical action plays the role of the phase $\phi = S_{Path}/\hbar$ associated with the path. The amplitude for a particle in a box to go from state $|i\rangle$ to state $|f\rangle$ is given by

$$\langle f|e^{-i\frac{Ht}{\hbar}}|i\rangle = \sum_{\text{Paths } i \to f} \exp\left[i\frac{S_{\text{path}}}{\hbar}\right]$$

where

$$S_{\text{path}} = \int_0^t dt' \Big(p\dot{q} - H[p,q]\Big) \tag{13.1}$$

The Feynman formulation is a precise reformulation of operator quantum mechanics. In the classical limit $\hbar \to 0$, the path integral is dominated by the paths of stationary phase, which correspond to the classical path which minimizes the action.

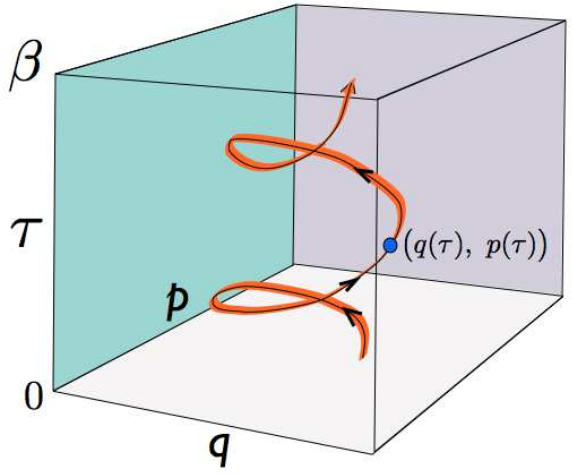


Figure 13.1: Illustrating a periodic path in imaginary time that contributes to the partition function of a single particle.

Feynman's idea can be extended to encompass statistical mechanics by treating the Boltzmann density matrix as a time-evolution operator in imaginary time. The trace over the density matrix is then the sum of amplitudes of paths that return to the initial configuration after an imaginary time $t = i\hbar\beta$:

$$Z = \text{Tr}\left[e^{-\beta\hat{H}}\right] = \sum_{\lambda}\langle\lambda|e^{-i\frac{Ht}{\hbar}}|\lambda\rangle\Big|_{t=-i\hbar\beta} \tag{13.2}$$

By changing variables to $it/\hbar \to \tau$, so that $idt/\hbar \to d\tau$, and $p\dot{q}dt \to pqd\tau$ we obtain we see that we can write this quantity as

$$Z = \sum_{\text{periodic paths}} \exp\left[-S_E\right]$$

where

$$S_E = \int_0^\beta d\tau \Big(-\frac{i}{\hbar}p\partial_\tau q + H[p,q]\Big). \tag{13.3}$$

We will now discuss a sophisticated extension of this idea to many body systems, in which the path integral sums over the configurations of the particle fields rather than the trajectories of the par-

ticles themselves. The key innovation that makes this possible, is the use of coherent states, which are literally, eigenstates of the quantum field. In quantum optics, such states, sometimes called "Glauber states", are used to describe "minimum-uncertainty" wave-packets of photon fields[4]. For a single boson field, a coherent state is given by

$$|b\rangle = e^{\hat{b}^\dagger b}|0\rangle \tag{13.4}$$

where in this chapter, we use the roman $\hat{b}$ and $\hat{b}^\dagger$ to denote boson operators, reserving the italic b and $\bar{b}$ for the corresponding eigenvalues. Now $|0\rangle$ is a harmonic oscillator ground-state defined by $\hat{b}|0\rangle = 0$, and it forms a a minimum uncertainty wavepacket centred around the origin of phase space. By contrast, the state $|b\rangle$ is the result of translating $|0\rangle$ so that it is centered around the point (q, p) in phase space, where $b = (q + ip)/\sqrt{2\hbar}$ incorporates both variables into a single complex variable (see problem 14.1). Paradoxically, though the state *is* an eigenstate of $\hat{b} = (\hat{q} + i\hat{p})/\sqrt{2\hbar}$, it is not an eigenstate of either $\hat{q}$ or $\hat{p}$. In a many body problem the fields $\hat{\psi}(x)$ are defined at at each point in space and in the corresponding coherent state $|\phi\rangle$

$$\hat{\psi}(x)|\phi\rangle = \phi(x)|\phi\rangle. \tag{13.5}$$

We can still use the definition (13.11) for a coherent state, but now

$$\hat{b}^\dagger = \int d^d x\, \hat{\psi}^\dagger(x)\phi(x), \tag{13.6}$$

coherently adds a boson to a condensate with wavefunction $\psi(x)$. (See example 12.33 and exercise 12.6.) These states are the "wavepackets" of many body physics. With care, we can use them as a basis set in which the matrix elements of the Hamiltonian are obtained simply by replacing the field operators by their expectation values. Using this procedure, the partition function can be re-written as a path integral in which $\phi(x, t)$ defines a "history", or path over which the field at point x evolves, and (Fig. 13.2),

$$Z = \sum_{\text{periodic paths}} e^{-S_E[\bar{\phi},\phi]}. \tag{13.7}$$

By convention, we denote the complex conjugate of $\phi(x)$ by $\bar{\phi}(x)$. In chapter 3, we introduced motivated particle field operators of particles as the quantization of the single particle wavefunction, identifying $\phi(x) \sim q$, $i\hbar\bar{\phi}^\dagger(x) \sim p$ as the corresponding canonical position and momenta co-ordinates. Using this analogy the many-body analog of the kinetic term in (14.3) is

$$-\frac{i}{\hbar}p\partial_\tau q \sim \bar{\phi}(x)\partial_\tau\phi(x), \tag{13.8}$$

so the many-body analogue of (13.3) is expected to take the form

$$S_E = \int_0^\beta d\tau d^3x\,[\bar{\phi}(x,\tau)\partial_\tau\phi(x,\tau) + H[\bar{\phi},\phi]]\,. \tag{13.9}$$

where H is the many-body Hamiltonian, with field operators replaced by the c-numbers ϕ and $\bar{\phi}$. Infact, as we'll see, this is precisely the form that is obtained when the quantum partition function is

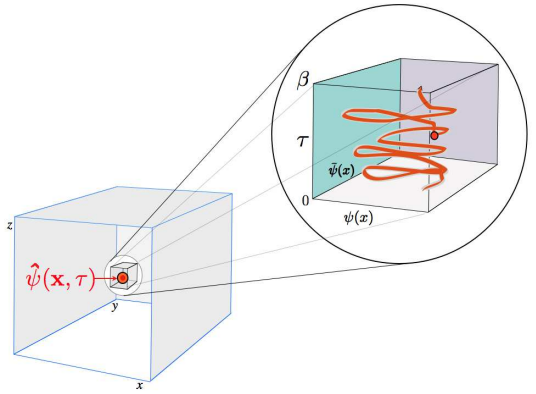


Figure 13.2: Illustrating how the operator field at each point in space is represented by a trajectory inside the path integral.

expanded in terms of coherent states $|\phi(x,\tau)\rangle$ [5, 6, 7]. Furthermore, time-ordered Green's functions can also be re-written as an average under the path integral, so that

$$\langle T\hat{\psi}(1)\hat{\psi}^\dagger(2)\rangle = \frac{1}{Z}\sum_{\text{path}} \exp\Big[-S_{\text{path}}\Big]\phi(1)\bar{\phi}(2)$$

where $\bar{\psi}(2)$ is the complex conjugate of $\psi(2)$. In this way, the quantum mechanics of the many body system is transformed from an operator formalism, into a *statistical* description, with each with each space-time configuration of the fields weighted by the action.

Remarkably, this approach can be extended to include fermions, using an idea of Julian Schwinger [8] that generalizies the concept of "c-numbers" to include anticommuting Grassman numbers. For fermions, the numbers $\psi(x)$ appearing in the coherent states must *anticommute* with each-other. They are thus a new kind of number, which requires some new algebraic tricks. Moreover, we'll see that that we can evaluate the corresponding path integral for *all* non-interacting problems. This is already a major achievement.

A final aspect of path integrals, is that interacting problems can be transformed, by the method of "Hubbard Stratonovich" [9, 10], into a problem of "free" particles moving in a fluctuating effective field. This technique provides an important tool for the study of broken symmetry phase transitions.

$$Z_{\text{interacting}} \to \sum_{\{\Delta\}}\Big[\text{path integral of fermions moving in field } \Delta\Big] \tag{13.10}$$

where $\{\Delta\}$ denotes a given configuration of the symmetry breaking field Δ.

13.2 Coherent states for Bosons

To demonstrate the path integral approach, and its derivation using coherent states, we will start with the bosonic path integral. As a warm up for path integrals, we need to establish a few key properties of the bosonic coherent state. We start by considering the coherent state of a single boson operator $\hat{b}^\dagger$, given by

$$|b\rangle = e^{\hat{b}^\dagger b}|0\rangle, \tag{13.11}$$

where b is a complex number. This state is an eigenstate of the annihilation operator

$$\hat{b}|b\rangle = b|b\rangle. \tag{13.12}$$

We can also form the conjugate state

$$\langle\bar{b}| = \langle 0|e^{\bar{b}\hat{b}}. \tag{13.13}$$

which is the eigenstate of the creation operator,

$$\langle\bar{b}|\hat{b}^\dagger = \langle\bar{b}|\bar{b},$$

where $\bar{b}$ is the complex conjugate of b. Although b and $\bar{b}$ are complex conjugates of one-another, they are derived from two independent real variables, and when we integrate over them we need a double integral in which we treat b and $\bar{b}$ as independent variables. The "bar" notation is adopted by convention to emphasize this linear independence.

A coherent state describes a condensate with an indefinite particle number. If we decompose it into eigenstates of particle number n by expanding in powers of b we obtain

$$|b\rangle = \sum_n \frac{b^n}{n!}(\hat{b}^\dagger)^n|0\rangle = \sum_n |n\rangle\frac{b^n}{\sqrt{n!}} \tag{13.14}$$

where $|n\rangle = \frac{(\hat{b}^\dagger)^n}{\sqrt{n!}}|0\rangle$ is the eigenstate of the number operator $\hat{n} = \hat{b}^\dagger\hat{b}$. In this way we see that the amplitude for a coherent state to be in a state with n particles is

$$\phi_n(b) = \langle n|b\rangle = \frac{b^n}{\sqrt{n!}}. \tag{13.15}$$

Similarly,

$$\langle\bar{b}| = \sum_m \frac{\bar{b}^m}{\sqrt{m!}}\langle m|, \tag{13.16}$$

and

$$\langle\bar{b}|m\rangle = \frac{\bar{b}^m}{\sqrt{m!}} \tag{13.17}$$

From (13.14) and (13.16), the overlap between the two states $\langle\bar{b}_1|$ and $|b_2\rangle$ is given by

$$\langle\bar{b}_1|b_2\rangle = \sum_{m,n}\frac{\bar{b}_1^m}{\sqrt{m!}}\overbrace{\langle m|n\rangle}^{\delta_{mn}}\frac{b_2^n}{\sqrt{n!}} = \sum_n \frac{(\bar{b}_1 b_2)^n}{n!} = e^{\bar{b}_1 b_2}. \tag{13.18}$$

13.2.1 Matrix elements and the completeness relation.

Remarkably, even though coherent states are non-orthogonal, they can be used to great effectiveness as a basis (an overcomplete basis), in which the field operators are diagaonal. There are two important properties of the coherent state that we shall repeatedly use to great advantage:

- **Matrix elements**. Matrix elements of normal ordered operators $O[\hat{b}^\dagger, \hat{b}]$ between two coherent states are obtained simply by replacing the operators $\hat{b}$ and $\hat{b}^\dagger$ by the c-numbers b and $\bar{b}$ respectively:

$$\langle\bar{b}_1|\hat{O}[\hat{b}^\dagger, \hat{b}]|b_2\rangle = O[\bar{b}_1, b_2]\times\langle\bar{b}_1|b_2\rangle = O[\bar{b}_1, b_2]\times e^{\bar{b}_1 b_2} \tag{13.19}$$

- **Completeness**.

  The unit operator can be decomposed in terms of coherent states as follows

$$\hat{1} = \sum_{\bar{b},b}|b\rangle\langle\bar{b}|, \tag{13.20}$$

  where[1]

$$\sum_{\bar{b},b} \equiv \int\frac{d\bar{b}db}{2\pi i}e^{-\bar{b}b} \tag{13.24}$$

  is the normalized measure for summing over coherent states.

We present a detailed derivation of these two results in appendix 14A, continuing now to use them to derive a path integral.

[1] *Note:* In quantum optics, one often encounters the "normalized" coherent or Glauber state,

$$|b,\bar{b}\rangle_N = \frac{1}{\sqrt{2\pi i}}e^{-\bar{b}\hat{b}+\hat{b}^\dagger b}|0\rangle = \frac{1}{\sqrt{2\pi i}}e^{-\bar{b}b/2}|b\rangle \tag{13.21}$$

This affords the advantage of a simpler completeness relation

$$\underline{1} = \int d\bar{b}db\,|b,\bar{b}\rangle_N\langle b,\bar{b}|_N, \tag{13.22}$$

but unfortunately, the matrix elements of normal ordered operators now assume a more complex form,

$$\langle b_1,\bar{b}_1|\hat{O}(\hat{b}^\dagger,\hat{b})|b_2,b_2\rangle_N = e^{\bar{b}_1 b_2-\bar{b}_1 b_1/2-\bar{b}_2 b_2/2}O(\bar{b},b). \tag{13.23}$$

The prefactor in this expression vanishes if $b_1 = b_2$, but our use of completeness in the derivation of the path integral forces us to include paths where b_2 and b_1 are completely independent. For this reason, while Glauber states are a useful mnemonic device for remembering completeness, this book chooses to use coherent states without the normalizing prefactor.

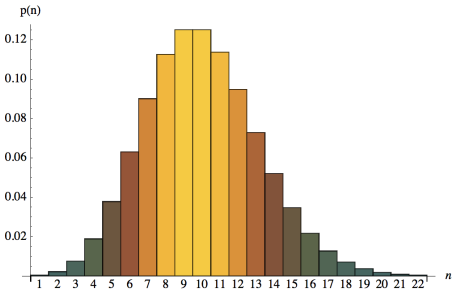


Figure 13.3: Probability distribution function for a coherent state with $\bar{b}b = n_0 = 10$.

Example 13.1: Prove that in a coherent state $|b\rangle$, the probability $p(n)$ to be in a state with n particles is a Poisson distribution with average particle number $n_0 = \langle \hat{n} \rangle = \bar{b}b$, and variance $\langle \delta n^2 \rangle = n_0$, where

$$p(n) = \frac{1}{n!}(\bar{b}b)^n e^{-\bar{b}b}, \tag{13.25}$$

Solution:

To calculate the normalized probalility to be in a state $|n\rangle$, we calculate

$$p(n) = \frac{|\langle n|b\rangle|^2}{\langle \bar{b}|b\rangle} = \frac{1}{n!}(\bar{b}b)^n e^{-\bar{b}b}.$$

The average particle number is

$$n_0 = \sum_{n=1,\infty} np(n) = \sum_{n=1,\infty} \frac{1}{n-1!}(\bar{b}b)^n e^{-\bar{b}b} = \bar{b}be^{-\bar{b}b} \sum_{n=0,\infty} \frac{1}{n!}(\bar{b}b)^n = \bar{b}b$$

Now

$$\langle \hat{n}^2 - \hat{n} \rangle = \sum_{n=1,\infty} n(n-1)p(n) = (\bar{b}b)^2 \sum_{n=2,\infty} \frac{1}{n-2!}(\bar{b}b)^{n-2} e^{-\bar{b}b} = (\bar{b}b)^2 = n_0^2$$

so that $\langle \hat{n}^2 \rangle = n_0(n_0+1)$ and hence $\langle \delta n^2 \rangle = \langle \hat{n}^2 \rangle - n_0^2 = n_0$. Notice that $\langle \delta n^2 \rangle / \langle n \rangle^2 = 1/n_0$. When n_0 is large, the distribution function becomes Gaussian and resembles a delta function in the thermodynamic limit.

Example 13.2: Using the completeness relation, prove that if $f(\alpha) = \langle f|\alpha\rangle$ is the overlap of

coherent state $|\alpha\rangle$ with state $|f\rangle$, then

$$f(\alpha) = \int \frac{d\bar{b}db}{2\pi i} f(b) e^{\bar{b}(\alpha - b)}. \tag{13.26}$$

Solution: Write the function $f(\alpha)$ as the overlap of state $\langle f|$ with state $|\alpha\rangle$, $f(\alpha) = \langle f|\alpha\rangle$. Now insert the completeness relation into this expression to obtain

$$\begin{aligned} \langle f|\alpha\rangle = \langle f|\hat{1}|\alpha\rangle &= \int \frac{d\bar{b}db}{2\pi i} \langle f|b\rangle\langle \bar{b}|\alpha\rangle e^{-\bar{b}b} \\ &= \int \frac{d\bar{b}db}{2\pi i} f(b) e^{\bar{b}(\alpha - b)}. \end{aligned} \tag{13.27}$$

Note the useful identity

$$\delta(\alpha - b) = \int \frac{d\bar{b}}{2\pi i} e^{\bar{b}(\alpha - b)}. \tag{13.28}$$

Example 13.3: Using the completeness relation, prove that the trace of any operator (not necessarily normal-ordered) $\hat{A}[\hat{b}^\dagger, \hat{b}]$ is given by

$$\mathrm{Tr}[A] = \sum_{\bar{b},b} \langle \bar{b}|A|b\rangle = \int \frac{d\bar{b}db}{2\pi i} e^{-\bar{b}b} \langle \bar{b}|A|b\rangle \tag{13.29}$$

Solution: In the particle-number basis, the trace over $\hat{A}$ is given by

$$\mathrm{Tr}[A] = \sum_n \langle n|A|n\rangle = \sum_{n,m} \langle m|A|n\rangle \delta_{nm} \tag{13.30}$$

From completeness,

$$\delta_{nm} = \sum_{\bar{b},b} \langle n|b\rangle\langle \bar{b}|m\rangle$$

so that

$$\begin{aligned} \mathrm{Tr}[A] &= \sum_{\bar{b},b,n,m} \langle n|b\rangle\langle \bar{b}|m\rangle\langle m|A|n\rangle \\ &= \sum_{\bar{b},b,m,n} \langle \bar{b}\, \overbrace{|m\rangle\langle m|}^{=1}\, \hat{A}\, \overbrace{|n\rangle\langle n|}^{=1}\, b\rangle \\ &= \sum_{\bar{b},b} \langle \bar{b}|A|b\rangle \equiv \int \frac{d\bar{b}db}{2\pi i} e^{-\bar{b}b} \langle \bar{b}|A|b\rangle \end{aligned} \tag{13.31}$$

Table. 1. Boson Calculus.

Completeness	$\langle b\|b\rangle = e^{\bar{b}b}$	Over-complete basis.
	$\int \frac{d\bar{b}db}{2\pi i} e^{-\bar{b}b}\|b\rangle\langle\bar{b}\| = \underline{1}$	Completeness relation.
	$\mathrm{Tr}[\hat{A}] = \int \frac{d\bar{b}db}{2\pi i} e^{-\bar{b}b}\langle\bar{b}\|\hat{A}\|b\rangle$	Trace Formula.
Gaussian Integrals	$\int \prod_j \frac{d\bar{b}_j db_j}{2\pi i} e^{-\left[\bar{b}\cdot A\cdot\bar{b} - \bar{j}\cdot b - \bar{b}\cdot j\right]} = \frac{e^{\left[\bar{j}\cdot A^{-1}\cdot j\right]}}{\det A}$	

13.3 Path integral for the partition function: Bosons

We now develop the path integral expression for the partition function of a single boson field, with a normal-ordered Hamiltonian $\hat{H}[\hat{b}^\dagger, \hat{b}]$. Our key result, to be derived is

$$\begin{aligned} Z &= \int \mathcal{D}[\bar{b}, b] e^{-S} \\ S &= \int_0^\beta d\tau \Big(\bar{b}\partial_\tau b + H[\bar{b}, b] \Big) \end{aligned} \tag{13.32}$$

Path integral for the Partition Function

All of our results can be simply generalized to include many different bosons. We begin by writing the trace required for the partition function in a coherent state basis, as

$$Z = \mathrm{Tr}[e^{-\beta H}] = \int \frac{d\bar{b}db}{2\pi i} e^{-\bar{b}b} \langle \bar{b}| e^{-\beta H}|b\rangle \tag{13.33}$$

Unfortunately, $e^{-\beta H[\hat{b}^\dagger, \hat{b}]}$ is not a normal-ordered operator, so we can't just replace the boson operators by their c-number equivalents. To achieve such a replacement, we divide the Boltzmann factor $e^{-\beta H} = U(\beta)$ (Fig 13.4) into a large number N tiny time-slices of duration $\Delta\tau = \beta/N$,

$$e^{-\beta H} = \left(e^{-\Delta\tau H}\right)^N \tag{13.34}$$

Since H is normal ordered, $e^{-\Delta\tau H} = 1 - \Delta\tau : H : + O(\Delta\tau^2)$ so that $e^{-\Delta\tau H}$ and $: e^{-\Delta\tau H} :$ only differ at second order in $\Delta\tau$. Thus, to an accuracy $O(\Delta\tau^2) = O(1/N^2)$ per time slice, we can replace the boson operators by c-numbers in each time slice.

$$\langle \bar{b}_j | e^{-\Delta\tau H[\hat{b}^\dagger, \hat{b}]} | b_{j-1}\rangle = \exp\left[\bar{b}_j b_{j-1} - \Delta\tau H[\bar{b}_j, b_{j-1}]\right] + (\Delta\tau^2). \tag{13.35}$$

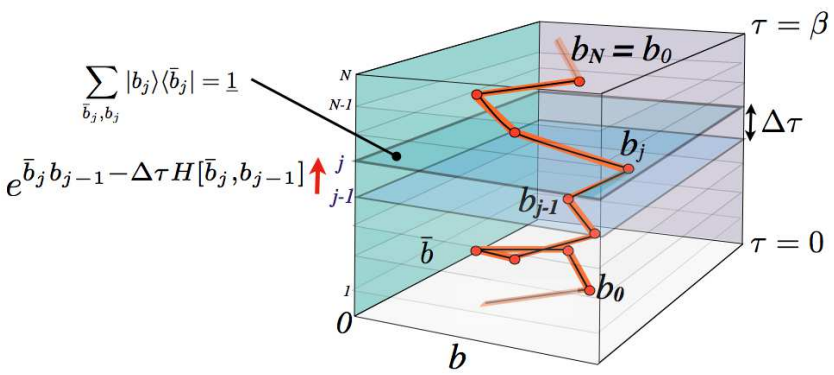


Figure 13.4: Illustrating the division of the trajectory into N time slices.

This is a huge step forward, which transforms the time-slice into a purely *algebraic* expression.

Let us now put this all together. The time-sliced partition function (13.33) is first written

$$Z = \int \frac{d\bar{b}_N db_0}{2\pi i} \langle \bar{b}_N | \left(e^{-\Delta\tau H}\right)^N |b_0\rangle e^{-\bar{b}_N b_0} \tag{13.36}$$

where we have relabelled $\bar{b} \to b_N$, $b \to b_0$ in (13.33). Next, between each time slice, we now introduce the completeness relation,

$$\hat{1} = \int \frac{d\bar{b}_j db_j}{2\pi i} |b_j\rangle e^{-\bar{b}_j b_j} \langle \bar{b}_j| \equiv \underline{1}_j. \tag{13.37}$$

so that the partition function becomes

$$\begin{aligned} Z &= \int \frac{d\bar{b}_N db_0}{2\pi i} \langle \bar{b}_N | e^{-\Delta\tau H} \times \ldots \underline{1}_j \times e^{-\Delta\tau H} \times \underline{1}_{j-1} \times \cdots \times \underline{1}_1 \times e^{-\Delta\tau H} |b_0\rangle e^{-\bar{b}_N b_0} \\ &= \int \mathcal{D}_N[\bar{b}, b] \prod_{j=1}^N e^{-\bar{b}_j b_j} \langle \bar{b}_j | e^{-\Delta\tau H} | b_{j-1}\rangle. \end{aligned} \tag{13.38}$$

Notice that we have identified $b_N \equiv b_0$ and $\bar{b}_N \equiv \bar{b}_0$. We have also introduced the short-hand notation

$$\mathcal{D}_N[\bar{b}, b] = \prod_{j=1}^N \frac{d\bar{b}_j db_j}{2\pi i} \tag{13.39}$$

for the measure.

Inserting expression (13.35) into (13.38), we then obtain

$$Z = \int \mathcal{D}_N[\bar{b}, b] \exp\left[-\sum_{j=1}^{N}\Big(\bar{b}_j(b_j - b_{j-1}) + \Delta\tau H[\bar{b}_j, b_{j-1}]\Big)\right] + O(N\Delta\tau^2), \tag{13.40}$$

where we have grouped the errors from all N time slices into a final term of order $O(N\Delta\tau^2) = O(1/N)$. Since this error vanishes in the limit $N \to \infty$, we may thus write

$$\begin{aligned} Z &= \lim_{N\to\infty} \int \mathcal{D}_N[\bar{b}, b] \exp[-S_N] \\ S_N &= \sum_{j=1}^{N} \Delta\tau \left(\bar{b}_j \frac{(b_j - b_{j-1})}{\Delta\tau} + H[\bar{b}_j, b_{j-1}]\right) \end{aligned} \tag{13.41}$$

This is the path integral representation of the partition function for a single boson field. Let us pause to reflect on this result. The integral represents a sum over all possible "histories" of the field,

$$\begin{aligned} b(\tau_j) &\equiv (b_1, b_2 \ldots b_N), \\ \bar{b}(\tau_j) &\equiv (\bar{b}_1, \bar{b}_2 \ldots \bar{b}_N), \end{aligned} \tag{13.42}$$

This kind of integral is also called a "functional integral", because it involves integrating over all values of the functions $b(\tau)$. When we take the thickness of each time slice to zero, the discrete functions $b(\tau_j) \equiv b_j$ become functions of continuous time. Our identification of $b_0 \equiv b_N$ and hence $\bar{b}_0 \equiv \bar{b}_N$ implies that the set of complete functions that we sum over is periodic in time:

$$b(\tau) = b(\tau + \beta), \qquad \bar{b}(\tau) = \bar{b}(\tau + \beta), \tag{13.43}$$

This is a new type of integral calculus - rather than integrating over all points on a line, we are integrating over all possible values of a function. We call these integrals "path integrals" or "functional integrals". Just as in conventional integral calculus, at some point we reserve a special notation for the continuum limit

$$\mathcal{D}_N[\bar{b}, b] \to \mathcal{D}[\bar{b}, b].$$

Assuming that the continuum limit is indeed a well-defined limit, we now replace

$$\begin{aligned} \sum_{j=1}^{N} \Delta\tau &\to \int_0^\beta d\tau, \\ b_j &\to b(\tau), \qquad \bar{b}_j \frac{(b_j - b_{j-1})}{\Delta\tau} \to \bar{b}\partial_\tau b, \\ H[\bar{b}_j, b_{j-1}] &\to H[\bar{b}, b]. \end{aligned} \tag{13.44}$$

These brash replacements hide a mountain of subtlety. Unlike a conventional integral, there is no sense of "continuity" associated with the field $b(\tau)$: inside the functional integral the paths we sum over are jagged noisy objects. However, if we look at their typical noise spectra, they have a

characteristic frequency. For a Harmonic oscillator, this is just the frequency of oscillation ω, but if we include interactions, there will typically be a spectrum of such frequencies with some minimum frequency ω_0. The continnum limit will develop provided $\omega_0\Delta\tau << 1$.

The limiting value of the path integral is then written

$$\begin{aligned} Z &= \int \mathcal{D}[\bar{z}, b] e^{-S} \\ S &= \int_0^\beta d\tau \Big(\bar{b}\partial_\tau b + H[\bar{b}, b]\Big) \end{aligned} \tag{13.45}$$

The simplest example of such a path integral is the non-interacting Harmonic oscillator, in which $H = \epsilon\hat{b}^\dagger\hat{b}$. For this case,

$$Z = \int \mathcal{D}[\bar{b}, b] \exp\left[-\int_0^\beta d\tau \bar{b}\Big(\partial_\tau + \epsilon\Big)b\right] \tag{13.46}$$

This is an example of a "Gaussian" path integral, because the action is just a quadratic function of the fields, and we'll shortly see that we can evaluate all such path integrals in a close form. It should be clear that this derivation does not depend on whether there are interaction terms in the Hamiltonian. We could equally well consider the case of the anharmonic oscillator, written in normal-ordered form as

$$H = \epsilon\hat{b}^\dagger\hat{b} + g : (\hat{b} + \hat{b}^\dagger)^4 :$$

The partition function for this case is now

$$Z = \int \mathcal{D}[\bar{b}, b] \exp\left[-\int_0^\beta d\tau \Big(\bar{b}(\partial_\tau + \epsilon)b + g(b + \bar{b})^4\Big)\right].$$

This is probably the simplest example of an "interacting" path integral.

13.3.1 Many bosons

The derivation of the last section is easily generalized to include many bosons, with a Hamiltonian $H[\hat{b}^\dagger_\lambda, \hat{b}_\lambda]$, by using a multi-variable coherent state

$$|b\rangle = \exp\left[\sum_\lambda \hat{b}^\dagger_\lambda b_\lambda\right].$$

Since this is just a product of coherent states, we can simply extend the completeness relationship as product of the measures for each individual boson

$$\hat{1} = \sum_{\bar{b},b} |b\rangle\langle b| \tag{13.47}$$

where now

$$\sum_{\bar{b},b} = \int \prod_\lambda \frac{d\bar{b}_\lambda db_\lambda}{2\pi i} e^{-\bar{b}_\lambda b_\lambda}$$

The procedure of developing the path integral is exactly the same: we subdivide the interval into N time slices, approximating $e^{-\Delta\tau H}$ by its normal ordered form. The resulting path integral is formally very similar,

$$\begin{aligned} Z &= \int \mathcal{D}[\bar{b}, b] e^{-S} \\ S &= \int_0^\beta d\tau \Big(\sum_\lambda \bar{b}_\lambda \partial_\tau b_\lambda + H[\bar{b}_\lambda, b_\lambda] \Big) \end{aligned} \tag{13.48}$$

Path integral for the partition function: many bosons.

where the measure is now a product of the measure for each boson field,

$$\mathcal{D}[\bar{b}, b] = \prod_\lambda \mathcal{D}[\bar{b}_\lambda, b_\lambda]$$

For example, the path integral for a gas of free bosons with Hamiltonian $H = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \hat{\mathrm{b}}^\dagger_{\mathbf{k}} \hat{\mathrm{b}}_{\mathbf{k}}$ has the action

$$S = \int_0^\beta \Big[\sum_{\mathbf{k}} \bar{b}_{\mathbf{k}} (\partial_\tau + \omega_{\mathbf{k}}) b_{\mathbf{k}} \Big].$$

13.3.2 Time-ordered expectation values

In addition to providing equilibrium thermodynamics, the path integral can also be used to calculate time-ordered expectation values. The division of time into N time-slices using coherent states can also be carried out for the evaluation of arbitrary time-ordered products of fields - and when we do so, we discover that the time-ordered product of fields maps onto a path integral over the corresponding c-number product of fields. Thus for the two-point Green's function

$$G(2-1) = -\langle T \hat{\mathrm{b}}(2) \hat{\mathrm{b}}^\dagger(1) \rangle = -\frac{\int \mathcal{D}[\bar{b}, b] e^{-S} b(2) \bar{b}(1)}{\int \mathcal{D}[\bar{b}, b] e^{-S}} \tag{13.49}$$

where we have used the notation $1 \equiv (\tau_1, X_1, \{\lambda_1\})$ to denote the continuous and discrete variables associated with the boson field. *In this way, time-ordered products of operators become weighted averages of c-numbers inside the path-integral*. The operator form for the Green's function is written in terms of the Heisenberg fields and to convert it into a path integral, we need to rewrite the Heisenberg field operators in terms of the Schrödinger fields,

$$\hat{\mathrm{b}}_H(2) = e^{H\tau_2} \hat{\mathrm{b}}_S(2) e^{-H\tau_2}$$

where the time argument τ_2 of the Schrödinger field $\hat{\mathrm{b}}_S(2)$ is a dummy variable. Now with this device, the Green's function can be transformed to the Schrödinger representation as follows

$$\begin{aligned} G(2-1) &= -\frac{1}{Z} \mathrm{Tr}[e^{-\beta H} T\Big\{ \hat{\mathrm{b}}_H(2) \hat{\mathrm{b}}^\dagger{}_H(1) \Big\}] \\ &= -\frac{1}{Z} \mathrm{Tr}[e^{-\beta H} T\Big\{ e^{\tau_2 H} \hat{\mathrm{b}}_S(2) e^{-\tau_2 H} e^{\tau_1 H} \hat{\mathrm{b}}^\dagger{}_S(1) e^{-\tau_1 H} \Big\}] \\ &= -\frac{1}{Z} \mathrm{Tr}[T\Big\{ U(\beta - \tau_2) \hat{\mathrm{b}}_S(2) U(\tau_2 - \tau_1) \hat{\mathrm{b}}^\dagger{}_S(1) U(\tau_1) \Big\}] \\ &= \mathrm{Tr}[T\Big\{ U(\beta) \hat{\mathrm{b}}_S(2) \hat{\mathrm{b}}^\dagger{}_S(1) \Big\}] \end{aligned} \tag{13.50}$$

where $U(\tau) = e^{-H\tau}$ is the time-evolution operator. To write the Green's function as a path integral, we now expand the time-ordered trace in terms of N time slices, introducing the Schrodinger operators at the time-slices τ_j and τ_k which corresponding to τ_1 and τ_2 respectively. Here's where coherent states work their marvellous magic, for we can rewrite the destruction operator as

$$\hat{\mathrm{b}}_S(\tau_k) = \hat{\mathrm{b}}_S(\tau_k) \times \underline{1}_k = \int \frac{d\bar{b}_k b_k}{2\pi i} e^{-\bar{b}_k b_k} |b_k\rangle \, b_k \langle \bar{b}_k| \tag{13.51}$$

and similarly

$$\hat{\mathrm{b}}^\dagger{}_S(\tau_j) = \underline{1}_j \times \hat{\mathrm{b}}^\dagger{}_S(\tau_j) = \int \frac{d\bar{b}_j b_j}{2\pi i} e^{-\bar{b}_j b_j} |b_j\rangle \, \bar{b}_j \, \langle \bar{b}_j|, \tag{13.52}$$

so that inside the path integral, $\hat{\mathrm{b}}_S(2) \hat{\mathrm{b}}^\dagger{}_S(1) \to b(2)\bar{b}(1)$ and

$$\mathrm{Tr}[T\Big\{ U(\beta) \hat{\mathrm{b}}_S(2) \hat{\mathrm{b}}^\dagger{}_S(1) \Big\}] = \int \mathcal{D}[\bar{b}, b] e^{-S} b(2) \bar{b}(1)$$

from which the path integral expression for the Green's function (13.49) follows. We can easily extend these results to all higher moments, quite generally, mapping time-ordered Green functions onto the corresponding moments under the path integral

$$\langle T \hat{\mathrm{b}}(1) \hat{\mathrm{b}}(2) \ldots \hat{\mathrm{b}}^\dagger(2') \hat{\mathrm{b}}^\dagger(1') \rangle = \frac{\int \mathcal{D}[\bar{b}, b] e^{-S} b(1) b(2) \ldots \bar{b}(2') \bar{b}(1')}{\int \mathcal{D}[\bar{b}, b] e^{-S}} \tag{13.53}$$

In this way, the path integral maps a system of interacting particles onto a statistical mechanics problem, with distribution function e^{-S}.

13.3.3 Gaussian path integrals

An important class of path integrals are the "Gaussian path integrals", in which the action is a quadratic functional of the fields. For example, for for free bosons Hamiltonian $\hat{H} = \hat{\mathrm{b}}^\dagger{}_\alpha h_{\alpha\beta} \hat{\mathrm{b}}_\beta$ the action is

$$S_E = \int_0^\beta d\tau \bar{b}_\alpha (\partial_\tau + h_{\alpha\beta}) b_\beta \equiv \int_0^\beta d\tau \bar{b} (\partial_\tau + \underline{h}) b \tag{13.54}$$

Remarkably, all Gaussian path integrals can be evaluated in a closed form and the key result is

$$\boxed{Z_G = \int \mathcal{D}[\bar{b}, b] \exp\left[-\int_0^\beta d\tau \bar{b}(\partial_\tau + \underline{h})b\right] = [\det(\partial_\tau + \underline{h})]^{-1}} \tag{13.55}$$

Bosonic Gaussian Integral

To understand this result, it is helpful to think of the function $b_\alpha(\tau) \equiv b_{\tilde{\alpha}}$ as a huge vector labelled by the indices $\tilde{\alpha} \equiv (\alpha, \tau)$. From this perspective, a Gaussian action is a vast matrix bilinear

$$S_E = \sum_{(\alpha,\tau),\ (\beta,\tau')} \bar{b}_\alpha(\tau) M_{\alpha\beta}(\tau,\tau') b_\beta(\tau') \equiv \bar{b} \cdot M \cdot b, \tag{13.56}$$

where

$$M_{\alpha\beta}(\tau,\tau') = \delta(\tau - \tau')(\partial_{\tau'} + h_{\alpha\beta}). \tag{13.57}$$

You may be worried about the notion of treating time-integration as a summation. To assuage your doubts, it is useful to re-write S_E in the frequency domain, where summations over time are replaced by discrete frequency summations. Since $b(\tau) = b(\tau + \beta)$, the Bose field can always be represented in terms of a discrete set of Fourier components,

$$b_\alpha(\tau) = \frac{1}{\sqrt{\beta}} \sum_n b_\alpha(i\nu_n) e^{i\nu_n \tau}. \tag{13.58}$$

In this basis

$$[\underline{M}(\tau - \tau')]_{\alpha\beta} = \delta(\tau - \tau')(\partial_{\tau'} + h_{\alpha\beta}) \longrightarrow (-i\nu_n \delta_{\alpha\beta} + h_{\alpha\beta}) = \underline{M}(i\nu_n) \tag{13.59}$$

so the action becomes a discrete summation over Matsubara frequencies

$$S_E = \sum_{i\nu_n} \bar{b}_\alpha(i\nu_n)\Big(-i\nu_n \delta_{\alpha\beta} + h_{\alpha\beta}\Big) b_\beta(i\nu_n) \equiv \bar{b} \cdot M \cdot b \tag{13.60}$$

To integrate a Gaussian path integral, we employ the general result for a multi-dimensional Gaussian integral

$$\boxed{\int \prod_\alpha \frac{d\bar{b}_\alpha db_\alpha}{2\pi i} e^{-\bar{b}_\alpha M_{\alpha\beta} b_\beta} = \frac{1}{\det[M]}} \tag{13.61}$$

where M is a matrix with non-zero eigenvalues. To prove this result we transform to a basis where M is explicitly diagonal. Let $b = U \cdot a$, and $\bar{b} = \bar{a} \cdot U^\dagger$, where $U \equiv U_{\alpha\lambda}$ is the unitary matrix that diagonalizes M, then since $U^\dagger{}_{\lambda\alpha} M_{\alpha\beta} U_{\beta\lambda'} = m_\lambda \delta_{\lambda\lambda'}$, where the m_λ are the eigenvalues of M,

$$\bar{b}_\alpha M_{\alpha\beta} b_\beta = \bar{a}_\lambda m_\lambda a_\lambda$$

is explicitly diagonal. Furthermore, under a unitary transformation, the measure remains unchanged. To see this, we write the transformed measure using a Jacobian,

$$\prod_\alpha d\bar{b}_\alpha db_\alpha = \prod_\alpha d\bar{a}_\alpha da_\alpha \times \frac{\delta[\bar{b}, b]}{\delta[\bar{a}, a]} = \prod_\alpha d\bar{a}_\alpha da_\alpha \left\| \begin{matrix} U^\dagger & 0 \\ 0 & U \end{matrix} \right\| = \prod_\alpha d\bar{a}_\alpha da_\alpha$$

where unitarity guarantees that the Jacobian is unity:

$$\left\| \begin{matrix} U^\dagger & 0 \\ 0 & U \end{matrix} \right\| = \mathrm{Det}[U^\dagger U] = 1.$$

Under these transformations, the Gaussian integral becomes diagonal and can be explicitly evaluated:

$$\int \prod_\alpha \frac{d\bar{b}_\alpha db_\alpha}{2\pi i} e^{-\bar{b}_\alpha M_{\alpha\beta} b_\beta} = \prod_\lambda \int \frac{d\bar{a}_\lambda da_\lambda}{2\pi i} e^{-m_\lambda \bar{a}_\lambda a_\lambda} = \Big(\prod_\lambda m_\lambda\Big)^{-1} = \frac{1}{\mathrm{Det}[M]} \tag{13.62}$$

where, in the last step, we have identified the determinant of M with the product of its eigenvalues, $\mathrm{Det}[M] = \prod_\lambda m_\lambda$. Finally, if we now replace $M \to \partial_\tau + h$, we obtain the general relationship given in (13.55).

$$Z_G = \frac{1}{\mathrm{Det}[\partial_\tau + \underline{h}]} \tag{13.63}$$

We can equally well write this in the frequency-domain, where the determinant can be explicitly evaluated:

$$Z_G = \int \mathcal{D}[\bar{b}, b] \exp\left[-\sum_n \bar{b}(i\nu_n)(-i\nu_n + \underline{h})b(i\nu_n)\right] = \frac{1}{\prod_n \mathrm{Det}(-i\nu_n + \underline{h})} = \frac{1}{\prod_{n,\lambda}(-i\nu_n + \epsilon_\lambda)} \tag{13.64}$$

where the ϵ_λ are the energy eigenvalues of $\underline{h}$. This expression is most usefully re-written as an expression for the Free energy

$$F_G = -T \ln Z_G = T \sum_n \mathrm{Tr}\ln(\underline{h} - i\nu_n) e^{i\nu_n 0^+} = T \sum_{n,\lambda} \ln(\epsilon_\lambda - i\nu_n) e^{i\nu_n 0^+}$$

where we have used the identity $\ln \mathrm{Det} A = \mathrm{Tr} \ln A$ and have introduced the convergence term $e^{i\nu_n 0^+}$. This term is motivated by the observation that derivatives of the partition function represent equal time expectation values, which are the expectation values of time-ordered operators at an infinitesimally negative time.

In ending this section, we make one last identification. For a diagonalized non-interacting Hamiltonian, the bosonic Green's function is given by

$$G_{\lambda\lambda'}(i\nu_n) = \delta_{\lambda\lambda'}(i\nu_n - \epsilon_\lambda)^{-1}. \tag{13.65}$$

So we can identify $(-i\nu_n + \epsilon_\lambda) = -G^{-1}(i\nu_n) = -G^{-1}$, as the inverse Green's function. Since this identity holds in any basis, we can identify $(\partial_\tau + \underline{h}) \equiv -G^{-1}$ in the time domain. An alternative expression for the Gaussian integral is then

$$Z_G = \int \mathcal{D}[\bar{b}, b] \exp\left[-\int_0^\beta \bar{b}(-G^{-1})b\right] = \frac{1}{\mathrm{Det}[-G^{-1}]} \tag{13.66}$$

If we take logarithms of both sides, we may write down the Free energy in terms of the one-particle Green's function

$$F = T \ln Det[-G^{-1}] = T \mathrm{Tr} \ln[-G^{-1}]. \tag{13.67}$$

This expression enables us to relate the Green's function and Free energy without having to first diagonalize the Hamiltonian G^{-1}.

Example 13.4: Use the equation of motion, $\partial_\tau \hat{b}(1) = [\hat{H}, \hat{b}(1)]$ to confirm that for a free system of bosons, where $\hat{H} = \hat{b}^\dagger \underline{h} \hat{b} \equiv \hat{b}^\dagger{}_\alpha h_{\alpha\beta} \hat{b}_\beta$, the Green's function is given by $G = -(\partial_\tau + \underline{h})^{-1}$.

Solution: The boson Green's function is given by

$$G(1-2) = -\langle T \hat{b}(1) \hat{b}^\dagger(2) \rangle \tag{13.68}$$

The time-dependence of the Green's function has two components - a smoothly varying term derived from the time-evolution of the bose field and a discontinuous term derived from the derivatives of the time-ordering operator. To see this, let us first expand the time-ordering operator in terms of θ functions,

$$G(1-2) = -\langle \hat{b}(1) \hat{b}^\dagger(2) \rangle \theta(\tau_1 - \tau_2) - \langle \hat{b}^\dagger(2) \hat{b}(1) \rangle \theta(\tau_2 - \tau_1) \tag{13.69}$$

If we now take the derivative w.r.t. time, we must take account of the discontinuity in the theta functions. Using , $\partial_\tau \theta(\tau_1 - \tau_2) = \delta(\tau_1 - \tau_2)$ and $\partial_\tau \theta(\tau_2 - \tau_1) = -\delta(\tau_1 - \tau_2)$, we obtain

$$\begin{aligned} \partial_\tau G(1-2) &= \Big(-\langle \hat{b}(1) \hat{b}^\dagger(2) \rangle \delta(\tau_1 - \tau_2) + \langle \hat{b}^\dagger(2) \hat{b}(1) \rangle \delta(\tau_1 - \tau_2) \Big) - \langle T \partial_\tau \hat{b}(1) \hat{b}^\dagger(2) \rangle \\ &= -\langle \overbrace{[\hat{b}(1), \hat{b}^\dagger(2)]}^{\delta(1-2)} \rangle \delta(\tau_1 - \tau_2) - \langle T \overbrace{\partial_\tau \hat{b}(1)}^{[H, \hat{b}(1)]} \hat{b}^\dagger(2) \rangle \\ &= -\delta(1-2) - \langle T [H, \hat{b}(1)] \hat{b}^\dagger(2) \rangle. \end{aligned} \tag{13.70}$$

where we have simplified the first term using the canonical commutation relations

$$\Big([\hat{b}(1), \hat{b}^\dagger(2)] \delta(\tau_1 - \tau_2) \Big)_{\alpha\beta} \equiv [\hat{b}_\alpha, \hat{b}^\dagger_\beta] \delta(\tau_1 - \tau_2) = \delta_{\alpha\beta} \delta(\tau_1 - \tau_2) \equiv \delta(1-2)_{\alpha\beta},$$

and used the equation of motion, $\partial_\tau b(1) = [H, b(1)]$. The commutator between the Hamiltonian and the boson field is

$$[H, \hat{b}(1)]_\alpha \equiv [H, \hat{b}_\alpha] = -[\hat{b}_\alpha, \hat{b}^\dagger_\lambda h_{\lambda\beta} \hat{b}_\beta] = -\overbrace{[\hat{b}_\alpha, \hat{b}^\dagger_\lambda]}^{\delta_{\alpha\lambda}} h_{\lambda\beta} \hat{b}_\beta = -h_{\alpha\beta} \hat{b}_\beta \equiv -[\underline{h} \cdot \hat{b}(1)]_\alpha$$

so putting this all together, we have

$$\partial_\tau G(1-2) = -\delta(1-2) - \underline{h} \cdot G(1-2) \tag{13.71}$$

or

$$(\partial_\tau + \underline{h}) G(1-2) = -\delta(1-2) \tag{13.72}$$

If we write this expression succinctly as

$$(\partial_\tau + \underline{h}) G = -1. \tag{13.73}$$

we see that

$$G = -(\partial_\tau + \underline{h})^{-1}. \tag{13.74}$$

If you are uncomfortable with treating integrals over the time-domain as a matrix multiplication, you can Fourier transform (13.71), writing

$$G(\tau - \tau') = T \sum_n G(i\nu_n) e^{-i\nu_n(\tau - \tau')} \tag{13.75}$$

so that $\partial_\tau \to -i\nu_n$ and then (13.73) becomes

$$(i\nu_n - \underline{h}) \cdot G(i\nu_n) = \underline{1} \tag{13.76}$$

and hence

$$G(i\nu_n) = (i\nu_n - \underline{h})^{-1}. \tag{13.77}$$

which is the Fourier transform of (13.74).

Example 13.5: Calculate the free energy of free bosonic gas, where $\hat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{b}^\dagger{}_{\mathbf{k}} \hat{b}_{\mathbf{k}}$ using the path integral method.

Solution: We begin by writing the action in the Frequency domain as

$$\begin{aligned} S_E &= -\sum_{\mathbf{k}, i\nu_n} b(\mathbf{k}, i\nu_n) G(\mathbf{k}, i\nu_n)^{-1} b(\mathbf{k}, i\nu_n) \\ G(\mathbf{k}, i\nu_n)^{-1} &= (i\nu_n - \epsilon_{\mathbf{k}}). \end{aligned} \tag{13.78}$$

The partition function is given by

$$e^{-\beta F} = \frac{1}{\det[-G^{-1}]} \tag{13.79}$$

so that

$$F = T \mathrm{lnDet}[-G^{-1}] = T \mathrm{Tr} \ln[-G^{-1}] = T \sum_{\mathbf{k}, i\nu_n} \ln(\epsilon_{\mathbf{k}} - i\nu_n) e^{i\nu_n 0^+}, \tag{13.80}$$

where we have introduced the convergence factor $e^{i\nu_n 0^+}$ and used the identity $\ln \mathrm{Det}[A] = \mathrm{Tr} \ln A$. Carrying out the frequency summation using complex contour methods, we have

$$F = -\sum_{\mathbf{k}} \oint \frac{dz}{2\pi i} n(z) \ln(\epsilon_{\mathbf{k}} - z) \tag{13.81}$$

where the integral is anticlockwise around the branch-cut on the real axis. This branch-cut runs out from $\omega = \epsilon_{\mathbf{k}}$ to positive infinity, with a discontinuity of 2π. Rewriting the integral along this discontinuity, we have

$$F = -\sum_{\mathbf{k}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} n(\omega) \overbrace{\Big[\ln(\epsilon_{\mathbf{k}} - \omega + i\delta) - \ln(\epsilon_{\mathbf{k}} - \omega - i\delta) \Big]}^{2\pi i \, \theta(\omega - \epsilon_{\mathbf{k}})} = -\sum_{\mathbf{k}} \int_{\epsilon_{\mathbf{k}}}^{\infty} d\omega n(\omega)$$

$$= -T\sum_{\mathbf{k}}\Big[\ln(1-e^{-\beta\omega})\Big]_{\epsilon_{\mathbf{k}}}^{\infty} = +T\sum_{\mathbf{k}}[\ln(1-e^{-\beta\epsilon_{\mathbf{k}}})] \tag{13.82}$$

13.3.4 Source terms in Gaussian integrals

Source terms provide a means of probing the correlations and fluctuations described by a path integral. For Gaussian path integrals, the result of introducing source terms can be evaluated to obtain

$$\begin{aligned} Z_G[\bar{j},j] &= \int \mathcal{D}[\bar{b},b]\exp\left\{-\int_0^\beta d1\Big[\bar{b}\left(\partial_\tau+\underline{h}\right)b-\bar{j}(1))\cdot b(1)-\bar{b}(1)\cdot j(1)\Big]\right\} \\ &= \frac{\exp\left[-\int_0^\beta d1d2\bar{j}(1)G(1-2)j(2)\right]}{\mathrm{Det}[\partial_\tau+\underline{h}]} \end{aligned} \tag{13.83}$$

Bosonic Gaussian Path Integral with source terms

where we have used the schematic notation $1\equiv(\tau_1,X_1,\{\lambda_1\})$, $2\equiv(\tau_2,X_2,\{\lambda_1\})$, to denote the time, position and all other relevant indices of the boson field and $\int_0^\beta d1=\sum_{\lambda_1}\int_0^\beta d\tau_1\int d^dX_1$ to denote the corresponding integration over continuous variables and summation over discrete quantum numbers. The expansion of the left and the right-hand sides of this expression as a power-series provide the Wick expansion of multi-particle Green's functions of the Boson field. Differentiating first the left and then the right-hand side with respect to $\bar{j}(1)$ we obtain

$$\frac{1}{Z_G[\bar{j},j]}\frac{\delta Z_G[\bar{j},j]}{\delta\bar{j}(1)} = \frac{\int D[\bar{b},b]e^{-S}b(1)}{\int D[\bar{b},b]e^{-S}} \equiv \langle\hat{\mathrm{b}}(1)\rangle = -\int_0^\beta d2G(1-2)j(2). \tag{13.84}$$

Taking second-derivatives and setting the source terms to zero we obtain

$$\frac{1}{Z_G[\bar{j},j]}\frac{\delta^2 Z_G[\bar{j},j]}{\delta\bar{j}(1)\delta j(2)}\bigg|_{\bar{j},\,j=0} = \frac{\int D[\bar{b},b]e^{-S}b(1)\bar{b}(2)}{\int D[\bar{b},b]e^{-S}} \equiv \langle T\hat{\mathrm{b}}(1)\hat{\mathrm{b}}^\dagger(2)\rangle_{\bar{j},j=0} = -G(1-2) \tag{13.85}$$

while higher-order differentials give us the Wick expansion,

$$\begin{aligned} \frac{1}{Z_G[\bar{j},j]}\frac{\delta^{2n}Z_G[\bar{j},j]}{\delta\bar{j}(1)\ldots\delta j(1')}\bigg|_{\bar{j},\,j=0} &= \\ (-1)^n\sum_P G(1-P_1')G(2-P_2')\ldots G(n-P_n') &= \frac{\int D[\bar{b},b]e^{-S}b(1)b(2)\ldots\bar{b}(2')\bar{b}(1')}{\int D[\bar{b},b]e^{-S}} \\ &\equiv \langle T\hat{\mathrm{b}}(1)\hat{\mathrm{b}}(2)\ldots\hat{\mathrm{b}}^\dagger(2')\hat{\mathrm{b}}^\dagger(1')\rangle. \end{aligned} \tag{13.86}$$

In this remarkable fashion, the correlation functions of non-interacting bosons in imaginary time are identified with the classic properties of Gaussian-distributed random variables.

To prove (13.84), we take (13.61) and shift the integration variables inside the integral

$$b\to b-M^{-1}j, \qquad \bar{b}\to\bar{b}-\bar{j}M^{-1}, \tag{13.87}$$

Under this simple shift, the measure remains unchanged, while the action term $\bar{b}\cdot M\cdot b$ becomes

$$\bar{b}\cdot M\cdot b\to(\bar{b}-\bar{j}M^{-1})\cdot M\cdot(b-M^{-1}j)=\bar{b}\cdot M\cdot b-(\bar{j}\cdot b+\bar{b}\cdot j)+\bar{j}\cdot M^{-1}\cdot j. \tag{13.88}$$

Since the integral is unchanged under this change of variables, it follows that

$$e^{-\bar{j}\cdot Mj}\int\prod_\alpha\frac{d\bar{b}_\alpha db_\alpha}{2\pi i}e^{-(\bar{b}_\alpha M_{\alpha\beta}b_\beta-\bar{j}_\alpha b_\alpha-\bar{b}_\alpha j_\alpha)} = \frac{1}{\mathrm{Det}[M]} \tag{13.89}$$

in other words,

$$\int\prod_\alpha\frac{d\bar{b}_\alpha db_\alpha}{2\pi i}e^{-(\bar{b}_\alpha M_{\alpha\beta}b_\beta-\bar{j}_\alpha b_\alpha-\bar{b}_\alpha j_\alpha)} = \frac{e^{\bar{j}\cdot M^{-1}j}}{\det[M]} \tag{13.90}$$

If we rewrite this expression by replacing $M\to -G^{-1}=(\partial_\tau+h)$, we obtain the key result (13.84). As usual, if you are uncomfortable with the change from discrete, to continuous variables, this procedure can first be carried out using the discrete variables in Fourier space, followed by an inverse Fourier transformation back into real space.

13.4 Fermions: Coherent states and Grassman mathematics

We now generalize the results of the last section to fermions, using Grassman numbers to set up a completely parallel derivation of the fermionic path integral in terms of coherent states.

Feynman's original derivation of path integrals applied purely to bosonic fields and its extension to fermions was begun in the 1950s. The idea of using anticommuting numbers, both as eigenvalues of fermion fields and as fermionic source terms was proposed in a seminal paper by Julian Schwinger in 1953[8]. Early proposals for path integrals for fermions were made by P. Matthews and Abdus Salam in 1955[11] and by David Candlin in 1956 [5]. The first explicit formulation of the fermionic action in terms of Grassman numbers, with a derivation using fermion coherent states was made by by J. L. Martin in 1959[6]. The mathematical foundations of fermionic path integrals were extensively developed in the 1960s by Felix Berezin[12] and the extension of the fermionic path integral to imaginary time and finite temperature was later provided by David Sherrington and Sam Edwards[7, 13]. However it is only in the last few decades that the method has become a commonly used tool in quantum many body physics.

To illustrate the basic approach, we shall consider a a single fermionic field $\hat{\mathrm{c}}^\dagger$. The coherent state for this field is

$$|c\rangle = e^{\hat{\mathrm{c}}^\dagger c}|0\rangle$$

and its conjugate is

$$\langle\bar{c}| = \langle 0|e^{\bar{c}\hat{\mathrm{c}}}.$$

In this text we've reserved roman symbols $\hat{c}^\dagger$ and $\hat{c}$ for the creation and annihilation operators, to delineate them from their expectation values $\bar{c}$ and c. Here c and $\bar{c}$ are anticommuting "Grassmann numbers". Note that in common usage the notation $c^\dagger$ is often used interchangeably to describe both the operator and its Grassman counterpart $\bar{c}$.

There are a number of caveats you need to remember about Grassmans. On the one hand, the quantities c and $\bar{c}$ are numbers which *commute* with all observables $\hat{O}$, $c\hat{O} = \hat{O}c$. On the other hand, to correctly represent the anticommuting algebra of the original Fermi fields, Grassman numbers *anticommute* amongst themselves *and* with other Fermi operators, so that

$$c\bar{c} + \bar{c}c = 0, \qquad c\hat{\psi} + \hat{\psi}c = 0, \tag{13.91}$$

But c must also anticommute with itself, which means that

$$c^2 = \bar{c}^2 = 0, \tag{13.92}$$

But how can we possibly deal with numbers which when squared, give zero? Though this seems absurd, we'll see that anticommuting or "Grassman" numbers do form a non-trivial calculus and that ultimately, the leap to this new type of number is no worst and no more remarkable than the jump from real, to complex numbers.

The main effect of the anticommuting properties of Grassmans is to drastically reduce the set of possible functions and the set of possible linear operations one can carry out on such functions. For example, the Taylor series expansion of Grassman functions has to truncate at first order in any particular variable. Thus a function of two variables, $f(\bar{c}, c)$

$$f[\bar{c}, c] = f_o + \bar{c}f_1 + \bar{f}_1 c + f_{12}\bar{c}c$$

only has four terms! The coherent state also truncates, so that

$$\begin{aligned} |c\rangle &= |0\rangle + \hat{c}^\dagger c|0\rangle \\ &= |0\rangle + |1\rangle c \end{aligned} \tag{13.93}$$

so that the overlap between the "n" fermion state ($n = 0, 1$) and the coherent state is given by

$$\langle n|c\rangle = c^n, \qquad (n = 0, 1)$$

To develop a path integral representation for fermions one needs to know how to carry out Grassman calculus. The key properties of Grassman algebra are summarized in table 1. In particular, you will notice that the *only* formal difference with bosons, is that the measure contains a different normalization

$$\sum_{\bar{b},b} = \int \frac{d\bar{b}db}{2\pi i} e^{-\bar{b}b} \to \sum_{\bar{c},\,c} = \int d\bar{c}dc e^{-\bar{c}c}, \tag{13.94}$$

that the trace formula contains an additional minus sign

$$\mathrm{Tr}[A]_B = \sum_{\bar{b},b} \langle \bar{b}|A|b\rangle \to \mathrm{Tr}[A]_F = \sum_{\bar{c},c} \langle -\bar{c}|A|c\rangle. \tag{13.95}$$

and that both the Jacobian and the Gaussian integral are the *inverses* of their bosonic counterpart.

13.4.1 Completeness and matrix elements

Coherent states are over-complete, for

$$\langle \bar{c}|c\rangle = \langle 0|(1 + \bar{c}\hat{c})(1 + \hat{c}^\dagger c)|0\rangle = 1 + \bar{c}c = e^{\bar{c}c}. \tag{13.96}$$

Notice the formal parallel with the overlap of bosonic coherent states. To derive the completeness relation, we start with the identity

$$\int d\bar{c}dc e^{-\bar{c}c} c^n \bar{c}^m = \delta_{nm}, \qquad (n, m = 0, 1) \tag{13.97}$$

then by writing $c^n = \langle n|c\rangle$, $\bar{c}^m = \langle \bar{c}|m\rangle$ we see that the overlap between the eigenstates $|n\rangle$ of definite particle number is given by

$$\delta_{nm} = \langle n|m\rangle = \int d\bar{c}dc e^{-\bar{c}c} \langle n|c\rangle\langle \bar{c}|m\rangle = \langle n| \int d\bar{c}dc e^{-\bar{c}c}\, |c\rangle\langle \bar{c}|\, |m\rangle \tag{13.98}$$

from which it follows that

$$\int d\bar{c}dc|c\rangle\langle \bar{c}|e^{-\bar{c}c} = |0\rangle\langle 0| + |1\rangle\langle 1| \equiv \underline{1}. \tag{13.99}$$

Completeness relation

Alternatively, we may write

$$\sum_{\bar{c},c} |c\rangle\langle \bar{c}| = \underline{1}$$

where

$$\sum_{\bar{c},\,c} \equiv \int d\bar{c}dc e^{-\bar{c}c} \tag{13.100}$$

is the measure for fermionic coherent states. The exponential factor $e^{-\bar{c}c} = 1/\langle \bar{c}|c\rangle$ provides the normalizing factor to take account of the over-completeness.

Matrix elements between coherent states are easy to evaluate. If an operator $A[\hat{c}^\dagger, \hat{c}]$ is *normal ordered*, then since the coherent states are eigenvectors of the quantum fields, it follows that

$$\langle \bar{c}|\hat{A}|c\rangle = \langle \bar{c}|c\rangle A[\bar{c}, c] = e^{\bar{c}c} A[\bar{c}, c], \tag{13.101}$$

i.e

$$\langle \bar{c}|\hat{A}|c\rangle = e^{\bar{c}c} \times \text{ c-number formed by replacing } A[\hat{c}^\dagger, \hat{c}] \to A[\bar{c}, c]. \tag{13.102}$$

This wonderful feature of coherent states enables us at a swoop, to convert normal-ordered operators into c-numbers.

Table. 2. Grassman Calculus .

Algebra	$c_1c_2 = -c_2c_1$	anticommute with Fermions and other Grassman numbers
	$c\hat{b} = \hat{b}c, \quad c\hat{\psi} = -\hat{\psi}c$	commute with bosons, anticommute with Fermi operators.
Functions	$f[\bar{c}, c] = f_o + \bar{c}f_1 + \bar{f}_1 c + f_{12}\bar{c}c$	Since $c^2 = 0$, truncate at linear order in each variable.
Calculus	$\partial f = -\bar{f}_1 - f_{12}\bar{c}$	Differentiation
	$\bar{\partial} f = f_1 + f_{12}c$	
	$\int dc \equiv \partial_c$	$\int dc1 = \partial_c 1 = 0$
		$\int dcc = \partial_c c = 1$
Completeness	$\langle c\|c\rangle = e^{\bar{c}c}$	Over-complete basis.
	$\int d\bar{c}dce^{-\bar{c}c}\|c\rangle\langle\bar{c}\| = \underline{1}$	Completeness relation.
	$\mathrm{Tr}[\hat{A}] = \int d\bar{c}dce^{-\bar{c}c}\langle -\bar{c}\|\hat{A}\|c\rangle$	Trace Formula.
Change of variable	$J\left(\frac{c_1 \ldots c_r}{\xi_1 \ldots \xi_r}\right) = \left\|\frac{\partial c_1 \ldots c_r}{\partial \xi_1 \ldots \xi_r}\right\|^{-1}$	Jacobian - inverse of Bosonic Jacobian.
Gaussian Integrals	$\int \prod_j d\bar{c}_j dc_j e^{-\left[\bar{c}\cdot A\cdot\bar{c} - \bar{j}\cdot c - \bar{c}\cdot j\right]} = \det A \times e^{\left[\bar{j}\cdot A^{-1}\cdot j\right]}$	

The last result we need is the trace of A. We might guess that the appropriate expression is

$$Tr[\hat{A}] = \sum_{\bar{c},c}\langle\bar{c}|\hat{A}|c\rangle$$

actually - this is almost right, but infact, it turns out that the anticommuting properties of the Grassmann's force us to introduce a minus sign into this expression

$$Tr[\hat{A}] = \sum_{\bar{c},c}\langle -\bar{c}|\hat{A}|c\rangle = \int d\bar{c}dce^{-\bar{c}c}\langle -\bar{c}|\hat{A}|c\rangle \qquad (13.103)$$

Grassman Trace formula

which we shall shortly see, gives rise to the antisymmetric boundary conditions of fermionic fields. To prove the above result, we rewrite (13.98) as

$$\delta_{nm} = \langle n|m\rangle = \int d\bar{c}dce^{-\bar{c}c}\langle -\bar{c}|m\rangle\langle n|c\rangle \qquad (13.104)$$

where the minus sign arises from anticommuting c and $\bar{c}$. We can now rewrite the trace as

$$\begin{aligned}\mathrm{Tr}A &= \sum_{n,m}\langle m|A|n\rangle\delta_{nm} \\ &= \sum_{n,m}\int d\bar{c}dce^{-\bar{c}c}\langle -\bar{c}|m\rangle\langle m|A|n\rangle\langle n|c\rangle \\ &= \int d\bar{c}dce^{-\bar{c}c}\langle -\bar{c}|\hat{A}|c\rangle \qquad (13.105)\end{aligned}$$

We shall make extensive use of the completeness and trace formulae (13.99) and (13.103) in developing the path integral. Both expressions are simply generalized to many fields c_j by making the appropriate change in the measure and by replacing $\bar{c}c$ in the exponent, by the dot product,

$$\begin{aligned}d\bar{c}dc &\rightarrow \prod_j d\bar{c}_j dc_j, \qquad (13.106)\\ \bar{c}c &\rightarrow \sum_j \bar{c}_j c_j.\end{aligned}$$

13.4.2 Path integral for the partition function: Fermions

This section very closely parallels the derivation of the bosonic path integral in section (13.3), but for completeness, we include all relevant steps. To begin with, we consider a single fermion, with Hamiltonian

$$H = \epsilon\hat{c}^\dagger\hat{c} \qquad (13.107)$$

Using the trace formula (13.103), the partition function

$$Z = \mathrm{Tr}e^{-\beta H} \qquad (13.108)$$

can be re-written in terms of coherent states as

$$Z = -\int d\bar{c}_N dc_1 e^{\bar{c}_N c_1} \langle \bar{c}_N | e^{-\beta H} | c_1 \rangle, \tag{13.109}$$

where the labeling anticipates the next step. Now we expand the exponential into a sequence of time-slices

$$e^{-\beta H} = \left(e^{-\Delta\tau H}\right)^N, \qquad \Delta\tau = \beta/N. \tag{13.110}$$

Between each time slice we introduce the completeness relation

$$\int d\bar{c}_j dc_{j+1} |c_{j+1}\rangle\langle \bar{c}_j| e^{-\bar{c}_j c_{j+1}} = 1 \tag{13.111}$$

so that

$$Z = -\int d\bar{c}_N dc_1 e^{\bar{c}_N c_1} \prod_{j=1}^{N-1} d\bar{c}_j dc_{j+1} e^{-\bar{c}_j c_{j+1}} \prod_{j=1}^{N} \langle \bar{c}_j | e^{-H\Delta\tau} | c_j \rangle \tag{13.112}$$

where the first integral is associated with the trace and the subsequent integrals with the $N-1$ completeness relations. Now if we define

$$c_1 = -c_{N+1} \tag{13.113}$$

we are able to identify the N th time slice with the 0 th the time-slice. In this way, the integral associated with the trace

$$-\int d\bar{c}_N dc_1 e^{\bar{c}_N c_1} \langle \bar{c}_N | \ldots | c_1 \rangle = \int d\bar{c}_N dc_{N+1} e^{-\bar{c}_N c_{N+1}} \langle \bar{c}_N | \ldots | c_1 \rangle \tag{13.114}$$

can be absorbed into the other $N-1$ integrals, and furthermore, we notice that the fields entering into the discrete path integral are *antiperiodic*.

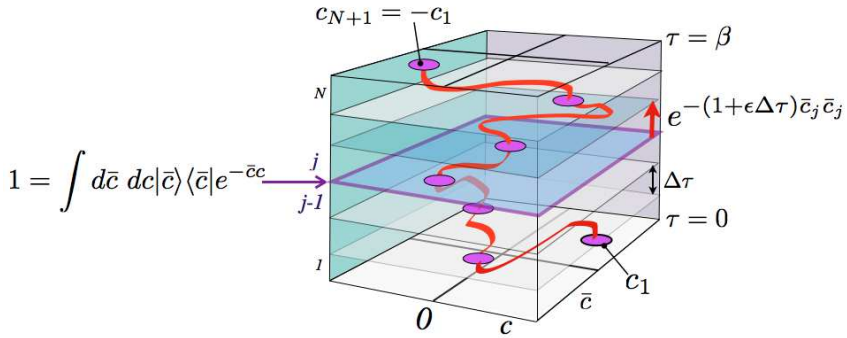
With this observation,

$$Z = \int \prod_{j=1}^{N} d\bar{c}_j dc_{j+1} e^{-\bar{c}_j c_{j+1}} \langle \bar{c}_j | e^{-H\Delta\tau} | c_j \rangle \tag{13.115}$$

Provided each time-slice is of sufficiently brief duration, we can replace $e^{-\Delta\tau H}$ by its normal ordered form, so that

$$\langle \bar{c}_j | e^{-H\Delta\tau} | c_j \rangle = e^{\bar{c}_j c_j} e^{-H[\bar{c}_j c_j]\Delta\tau} + O(\Delta\tau^2), \tag{13.116}$$

where $H[\bar{c}, c] = \epsilon \bar{c} c$ is the normal-ordered Hamiltonian, with Grassman numbers replacing operators.



Division of Grassmanian time evolution into "time-slices".

Combining (13.109) and (13.112) we can write

$$\begin{aligned} Z &= \mathrm{Lt}_{N\to\infty} Z_N \\ Z_N &= \int \prod_{j=1}^{N} d\bar{c}_j dc_j \exp\Big[-S\Big] \\ S &= \sum_{j=1}^{N} \Big[\bar{c}_j (c_{j+1} - c_j)/\Delta\tau + \epsilon \bar{c}_j c_j\Big]\Delta\tau, \end{aligned} \tag{13.117}$$

As in the bosonic case, this path integral represents a sum over all possible values "histories" of the fields:

$$c(\tau_j) \equiv \{c_1, c_2 \ldots c_N\}, \tag{13.118}$$

$$\bar{c}(\tau_j) \equiv \{\bar{c}_1, \bar{c}_2 \ldots \bar{c}_N\} \tag{13.119}$$

as illustrated in Fig. 2. This kind of integral is also called a "functional integral", because it involves integrating over all possible values of the functions $c(\tau)$ and $\bar{c}(\tau)$. When we take the thickness of the time slices to zero, the discrete functions $c(\tau)$ and $\bar{c}(\tau)$ become functions of continuous time. The boundary condition (13.113) implies that the set of complete functions which we sum over must satisfy anti-periodic boundary conditions

$$c(\tau + \beta) = -c(\tau), \qquad \bar{c}(\tau + \beta) = -\bar{c}(\tau)$$

In the continuum limit, $N \to \infty$, we now replace

$$\begin{aligned} \bar{c}_j (c_j - c_{j-1})/\Delta\tau &\to \bar{c}\partial_\tau c, \\ \sum_j \Delta\tau &\to \int_0^\beta d\tau. \end{aligned} \tag{13.120}$$

The sense in which c_j becomes "close" to c_{j+1} needs to be carefully understood. Suppose we rewrite the antiperiodic c_j in terms of their frequency components as

$$c_j = \frac{1}{\sqrt{\beta}} \sum_{|n|\leq N/2} c(i\omega_n) e^{-i\omega_n \tau_j},$$

then in this new basis,

$$\sum_j \bar{c}_j (c_{j+1} - c_j) = \sum_{|n|\leq N/2} \bar{c}(i\omega_n) \left[\frac{e^{-i\omega_n \Delta\tau} - 1}{\Delta\tau} \right] c(i\omega_n)$$

In practice, the path-integral is dominated by functions c_j with a maximum characteristic temporal frequency $max(|\omega_n|) \sim \epsilon$, so that as $\Delta\tau \to 0$, we can replace

$$\left[\frac{e^{-i\omega_n \Delta\tau} - 1}{\Delta\tau} \right] \to -i\omega_n$$

which is the Fourier transform of ∂_τ.

With these provisos, the continuum limit of the action and path integral are then

$$\begin{aligned} S &= \int_0^\infty d\tau \Big[\bar{c}(\partial_\tau + \epsilon) c \Big], \\ Z &= \int \mathcal{D}[\bar{c}, c] \exp\Big[-S \Big] \end{aligned} \tag{13.121}$$

where we use the notation

$$\mathcal{D}[\bar{c}, c] = \prod_{\tau_l} d\bar{c}(\tau_l) dc(\tau_l)$$

At first sight, it might seem a horrendous task to carry out the integral over all possible functions $c(\tau)$. How can we possibly do this in a controlled fashion? The clue to this problem lies in the observation that the set of functions $c(\tau)$ (and its conjugate, $\bar{c}(\tau)$) are spanned by a *discrete* but complete set of anti-periodic functions, as follows

$$c(\tau) = \frac{1}{\sqrt{\beta}} \sum_n c_n e^{-i\omega_n \tau},$$

We can integrate over all possible functions $c(\tau)$ by integrating over all possible values of the coefficients c_n and since the transformation which links these two bases is unitary, the Jacobian which links the two bases is unity, i.e.

$$\mathcal{D}[\bar{c}, c] \equiv \prod_n d\bar{c}_n dc_n$$

It is much easier to visualize and work with a discrete basis. We can transform to this basis, by replacing $\partial_\tau \to -i\omega_n$ in the action, rewriting it as

$$S = \sum_n \bar{c}_n (-i\omega_n + \epsilon) c_n$$

Now the path integral is just a discrete Gaussian integral

$$Z = \int \prod_n d\bar{c}_n dc_n \exp\Big[-\sum_n \bar{c}_n (-i\omega_n + \epsilon) c_n \Big] = \prod_n (-i\omega_n + \epsilon)$$

so that the Free energy is given by

$$F = -T \ln Z = -T \sum_n \ln(\epsilon - i\omega_n) e^{i\omega_n 0^+}$$

Here we have added a small convergence factor $e^{i\omega_n 0^+}$ because the time-evolution from $\tau = 0$ to $\tau = \beta$ is equivalent to time evolution from $\tau = 0$ to $\tau = 0^-$.

We can show that this reverts to the standard expression for one-particle free energy by replacing the Matsubara sum with a contour integral:

$$F = T \oint \frac{dz}{2\pi i} f(z) \ln[\epsilon_\lambda - z] e^{z0^+} \tag{13.122}$$

where the contour integral passes counter-clockwise around the poles of the Fermi function at $z = i\omega_n$, and the choice of $f(z)$ is dictated by the convergence factor. We take the logarithm to have a branch cut which extends from $z = \epsilon_\lambda$ to infinity. By deforming the integral around this branch cut we obtain

$$\begin{aligned} F &= -\int_\epsilon^\infty \frac{d\omega}{2\pi i} f(\omega) \Big[\ln(\epsilon - \omega - i\delta) - (\text{c.c.}) \Big] \\ &= \int_\epsilon^\infty d\omega f(\omega) \\ &= -T \ln[1 + e^{-\beta\epsilon}] \end{aligned} \tag{13.123}$$

which is the well-known Free energy of a single fermion.

Of course, here we have used a sledge-hammer to crack a walnut, but the virtue of the method is the ease with which it can be generalized to more complex problems. Three important points need to be made about this result:

- This result can easily be generalized to an arbitrary number of Fermi-fields. In this case,

  $$S = \int_0^\infty d\tau \Big[\sum_\lambda \bar{c}_\lambda \partial_\tau c_\lambda + H[\bar{c}, c] \Big],$$

  and the measure for the path integral becomes

  $$\mathcal{D}[\bar{c}, c] = \prod_{\tau_l, r} d\bar{c}_\lambda(\tau_l) dc_\lambda(\tau_l)$$

- The derivation did not depend on any details of H, and can thus be simply generalized to interacting Hamiltonians. In both cases, the conversion of the normal-order Hamiltonian occurs by simply replacing operators with the appropriate Grassman variables.

  $$: H[\hat{c}^\dagger, \hat{c}] : \to H[\bar{c}, c]$$

- Because the Jacobian for a unitary transformation is unity, we can change basis inside the path integral. For example, if we start with the action for a gas of fermions

$$S = \int_0^\beta d\tau \sum_{\mathbf{k}} \bar{c}_{\mathbf{k}}(\partial_\tau + \epsilon_{\mathbf{k}})c_{\mathbf{k}},$$

where $\epsilon_{\mathbf{k}} = (k^2/2m) - \mu$, we can transform to a completely discrete basis by Fourier transforming in time,

$$\begin{aligned} c_{\mathbf{k}} &= \frac{1}{\sqrt{\beta}}\sum_n c_{\mathbf{k}n}e^{i\omega_n\tau}, \\ \partial_\tau &\to -i\omega_n \\ \mathcal{D}[\bar{c},c] &\to \prod_{\mathbf{k},n} d\bar{c}_{\mathbf{k}n}dc_{\mathbf{k}n}. \end{aligned} \tag{13.124}$$

In the this discrete basis, the action becomes

$$S = \sum_{\mathbf{k},n}(\epsilon_{\mathbf{k}} - i\omega_n)\bar{c}_{\mathbf{k}n}c_{\mathbf{k}n}$$

This basis usually proves very useful for practical calculations.

- We can also transform to a continuum real-space basis, as follows

$$\begin{aligned} c_{\mathbf{k}} &= \frac{1}{\sqrt{V}}\int d^3x\psi(\mathbf{x})e^{-i\mathbf{k}\cdot\mathbf{x}}, \\ \epsilon_{\mathbf{k}} &\to -\frac{\nabla^2}{2m} - \mu \\ \mathcal{D}[\bar{c},c] &\to \mathcal{D}[\bar{\psi},\psi]. \end{aligned} \tag{13.125}$$

In the new basis, the the action becomes

$$S = \int_0^\beta d\tau \int d^3x\bar{\psi}(\mathbf{x})\Big[\partial_\tau - \frac{\nabla^2}{2m} - \mu\Big]\psi(\mathbf{x}).$$

The discrete and continuous measures, (13.124) and (13.125) are equivalent

$$\prod_{\mathbf{k},n} d\bar{c}_{\mathbf{k}n}dc_{\mathbf{k}n} \equiv \mathcal{D}[\bar{\psi},\psi].$$

because the space of continuous functions $\psi(x)$ is spanned by a complete, but discrete set of basis functions.

$$\psi(\mathbf{x},\tau) = \frac{1}{\sqrt{\beta V}}\sum_{\mathbf{k},n} c_{\mathbf{k}n}e^{i(\mathbf{k}\cdot\mathbf{x}-\omega_n\tau)},$$

We can integrate over all possible functions $\psi(\mathbf{x},\tau)$ by integrating over all values of the discrete vector $c_{\mathbf{k}n}$.

13.4.3 Gaussian Path Integral for Fermions

For non-interacting fermions the action only involves bilinears of the Fermi fields, so the path integral is of Gaussian form and can always be evaluated. To discuss the most general case, we shall include "source terms" in the original Hamiltonian, writing

$$H(\tau) = \sum_\lambda [\epsilon_\lambda \hat{c}_\lambda^\dagger \hat{c}_\lambda - \bar{j}_\lambda(\tau)\hat{c}_\lambda - \hat{c}_\lambda^\dagger j_\lambda(\tau)]$$

where $\hat{c}_\lambda^\dagger$ is Schrödinger field that creates a fermion in the eigenstate with energy ϵ_λ. With source terms, the partition function becomes a "generating functional"

$$Z[\bar{j},j] = \mathrm{Tr}\Big[\mathrm{T}\exp\{-\int_0^\beta d\tau H(\tau)\}\Big].$$

Derivatives of the generating functional generate the irreducible Green's functions of the fermions, for instance,

$$\frac{\delta \ln Z[\bar{j},j]}{\delta\bar{j}(1)} = \langle c(1)\rangle \tag{13.126}$$

$$\frac{\delta^2 \ln Z[\bar{j},j]}{\delta\bar{j}(2)\delta j(1)} = \langle T[c(1)c^\dagger(2)]\rangle - \langle c(2)\rangle\langle c^\dagger(1)\rangle \tag{13.127}$$

where

$$\langle \ldots\rangle = \frac{1}{Z[\bar{j},j]}\mathrm{Tr}\Big[\mathrm{T}\exp\{-\int_0^\beta d\tau H(\tau)\}\ldots\Big]$$

Transforming to a path integral representation, now

$$Z[\bar{j},j] = \int \mathcal{D}[\bar{c},c]e^{-S} \tag{13.128}$$

$$S = \int d\tau\Big[\bar{c}(\tau)(\partial_\tau + \underline{h})c(\tau) - \bar{j}(\tau)c(\tau) - \bar{c}(\tau)j(\tau)\Big] \tag{13.129}$$

where $\underline{h}_{\alpha\beta} = \epsilon_\alpha\delta_{\alpha\beta}$ is the one-particle Hamiltonian. One can carry out functional derivatives on this integral without actually evaluating it. For example, we find that

$$\langle c(1)\rangle = \frac{1}{Z[\bar{j},j]}\int \mathcal{D}[\bar{c},c]c(1)e^{-S} \tag{13.130}$$

$$\langle T[c(1)c^\dagger(2)]\rangle = \frac{1}{Z[\bar{j},j]}\int \mathcal{D}[\bar{c},c]c(1)\bar{c}(2)e^{-S} \tag{13.131}$$

Notice how the path integral automatically furnishes us with time-ordered expectation values.

Fortunately, the path integral is Gaussian, allowing us to use the general result obtained in Appendix 14D,

$$\int\prod_j d\bar{\xi}_j d\xi_j \exp[-\bar{\xi}\cdot A\cdot\xi + \bar{j}\cdot\xi + \bar{\xi}\cdot j] = \det A\exp[\bar{j}\cdot A^{-1}\cdot j]. \tag{13.132}$$

In the case considered here, $A = \partial_\tau + \underline{h}$, so we can do the integral, to obtain

$$\boxed{\begin{aligned} Z[\bar{j}, j] &= \int \mathcal{D}[\bar{c}, c] \exp\left[\int d\tau \Big[\bar{c}(\tau)(\partial_\tau + \underline{h})c(\tau) - \bar{j}(\tau)c(\tau) - \bar{c}(\tau)j(\tau)\Big]\right] \\ &= \det[\partial_\tau + \underline{h}] \exp\Big[-\int d\tau d\tau' \bar{j}(\tau)\underline{G}[\tau - \tau']j(\tau')\Big] \end{aligned}} \quad (13.133)$$

where $-(\partial_\tau + \underline{h})^{-1} = \underline{G}[\tau - \tau']$.

By differentiating (13.133) with respect to j and $\bar{j}$, we are able to identify

$$\left.\frac{\delta^2 \ln Z}{\delta \bar{j}(\tau)\delta j(\tau')}\right|_{\bar{j}, j=0} = \langle c(\tau)c^\dagger(\tau')\rangle = -\underline{G}[\tau - \tau'], \quad (13.134)$$

so the inverse of the Gaussian coefficient in the action $-[\partial\tau + \underline{h}]^{-1}$ directly determines the imaginary time Green-function of these non-interacting fermions. Higher order moments of the generating functional provide a derivation of Wick's theorem.

From the partition function in (13.133), the Free energy is then given by

$$F = -T\ln Z = -T\,\mathrm{lndet}[\partial_\tau + \underline{h}] = -T\,\mathrm{Trln}[\partial_\tau + \underline{h}] = T\,\mathrm{Trln}[-G^{-1}]$$

where we have used the result $\mathrm{lndet}[A] = \mathrm{Trln}[\partial_\tau + \underline{h}]$.

To explicitly compute the Free energy it is useful to transform to Fourier components,

$$\begin{aligned} c_\lambda(\tau) &= \frac{1}{\sqrt{\beta}}\sum_n c_{\lambda n} e^{-i\omega_n \tau}, \\ j_\lambda(\tau) &= \frac{1}{\sqrt{\beta}}\sum_n j_{\lambda n} e^{-i\omega_n \tau}, \end{aligned} \quad (13.135)$$

In this basis,

$$\begin{aligned} (\partial_\tau + \epsilon_\lambda) &\rightarrow (-i\omega_n + \epsilon_\lambda) \\ \underline{G} = -(\partial_\tau + \epsilon_\lambda)^{-1} &\rightarrow (i\omega_n - \epsilon_\lambda)^{-1} \end{aligned} \quad (13.136)$$

so that

$$S = \sum_{\lambda,n}\Big[[-i\omega_n + \epsilon_\lambda]\bar{c}_{\lambda n}c_{\lambda n} - \bar{j}_{\lambda n}c_{\lambda n} - \bar{c}_{\lambda n}j_{\lambda n}\Big] \quad (13.137)$$

whereupon,

$$\begin{aligned} \det[\partial_\tau + \underline{h}] &= \prod_{\lambda,n}(-i\omega_n + \epsilon_\lambda) \\ Z[\bar{j}, j] &= \prod_{\lambda,n}(-i\omega_n + \epsilon_\lambda)\exp\Big[\sum_{\lambda,n}(-i\omega_n + \epsilon_\lambda)^{-1}\bar{j}_{\lambda n}j_{\lambda n}\Big] \end{aligned} \quad (13.138)$$

If we set $j = 0$ in Z we obtain the Free energy in terms of the Fermionic Green function.

$$F = -T\sum_{\lambda,n}\ln[-i\omega_n + \epsilon_\lambda]$$

As in the case of a single field, by replacing the Matsubara sum with a contour integral we obtain

$$\begin{aligned} F &= T\sum_\lambda \oint \frac{dz}{2\pi i} f(z)\ln[\epsilon_\lambda - z] \quad (13.139) \\ &= -T\sum_\lambda \ln[1 + e^{-\beta\epsilon_\lambda}] \quad (13.140) \end{aligned}$$

If we differentiate Z with respect to its source terms, we obtain the Green's function:

$$-\frac{\delta^2 \ln Z}{\delta\bar{j}_{\lambda n}\delta j_{\lambda' n'}} = [\underline{G}]_{\lambda n, \lambda' n'} = \delta_{\lambda\lambda'}\delta_{nn'}\frac{1}{i\omega_n - \epsilon_\lambda}$$

13.5 Effective action and Hubbard Stratonovich transformation

13.5.1 Heuristic derivation

The "Hubbard Stratonovich" transformation [9, 10], provides a means of representing the interactions between fermions in terms of an exchange boson. It is in essence, a way of replacing an instantaneous interaction by a force-carrying boson that describes the fluctuations of an emergent order parameter. Using this method it becomes possible to formally "integrate out" the microscopic fermions, rewriting the problem as an effective field theory describing the thermal and quantum fluctuations of the order parameter as a path integral with a new "effective action". The method also provides an important formal basis for the order-parameter and mean-field description of broken symmetry states.

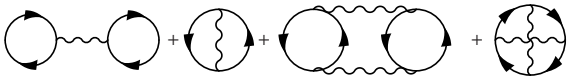
To motivate this approach, we begin with a heuristic derivation. Consider a simple attractive point interaction between particles $V(\mathbf{x} - \mathbf{x}') = -g\delta(\mathbf{x} - \mathbf{x}')$, given by the interaction Hamiltonian

$$H_I = -\frac{g}{2}\int_{\mathbf{x}} \rho(\mathbf{x})^2. \quad (13.141)$$

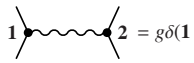
We can write the partition function as a path integral,

$$Z = \int \mathcal{D}[\psi]\exp\left[-\int_{\mathbf{x},\tau}\bar{\psi}(x)(\partial_\tau + \underline{h})\psi(x) - \frac{g}{2}\rho(x)^2\right] \quad (13.142)$$

If we expand the logarithm of the partition function diagrammatically, then we get a series of linked-cluster diagrams,

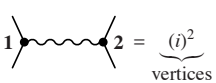
$\ln(Z/Z_0) =$  $+\ldots$ (13.143)

where the point interaction is represented by Feynman diagram



$$= g\delta(\mathbf{1}-\mathbf{2}). \tag{13.144}$$

Rather that thinking of an instantaneous contact interaction, we can regard this diagram as the exchange of force carrying boson, writing the diagram as



$$= \underbrace{(i)^2}_{\text{vertices}} \times \overbrace{-g\delta(\mathbf{1}-\mathbf{2})}^{-\langle T\phi(1)\phi(2)\rangle} \tag{13.145}$$

where the vertices $(-i)$ derive from an interaction $S_I' = \int_{\mathbf{x},\tau} \rho(x)\phi(x)$, between the fermions and the boson with imaginary time Green's function

$$G(\mathbf{1}-\mathbf{2}) = -\langle T\phi(\mathbf{1})\phi(\mathbf{2})\rangle = -g\delta(\mathbf{1}-\mathbf{2}) \tag{13.146}$$

But this implies that the exchange boson has a white noise correlation function $\langle T\phi(\mathbf{1})\phi(\mathbf{2})\rangle = \delta(\mathbf{1}-\mathbf{2})$: these kind of white noise correlations are exactly what we expect for a field governed by a simple Gaussian path integral, where

$$\frac{\int D[\phi]\phi(\mathbf{1})\phi(\mathbf{2})e^{-S_\phi}}{\int D[\phi]e^{-S_\phi}} = g\delta(\mathbf{1}-\mathbf{2}) \tag{13.147}$$

with the Gaussian action

$$S_\phi = \int_{\mathbf{x}}\int_0^\beta d\tau \frac{\phi(x)^2}{2g}. \tag{13.148}$$

By adding $S_\phi + S_I'$ to the free fermion action we can thus represent original point interaction by a fluctuating white-noise potential

$$-\frac{g}{2}\rho(x)^2 \to \rho(x)\phi(x) + \frac{\phi(x)^2}{2g}. \tag{13.149}$$

If we now insert this transformed interaction into the action, the transformed path integral expression of the partition function becomes

$$Z = \int \mathcal{D}[\psi,\phi]\exp\Big[-\int_{\mathbf{x},\tau}\bar\psi(x)[\partial_\tau + \underline{h} + \phi(x)]\psi(x) + \frac{1}{2g}\phi(x)^2\Big]. \tag{13.150}$$

Note that:

- Although our derivation is heuristic, we shall shortly see that the Hubbard Stratonovich transformation is *exact* so long as we allow $\phi(x) = \phi(\mathbf{x},\tau)$ to describe a fluctuating quantum variable inside the path integral.

- If we replace $\phi(\mathbf{x},\tau)$ by its average value, $\phi(\mathbf{x},\tau) \to \langle\phi(\mathbf{x},\tau)\rangle = \phi(\mathbf{x})$ we obtain a "mean-field theory". Suppose, instead of carrying out the Hubbard Stratonovich transformation, we chose to expand the density in powers of its fluctuations $\delta\rho(x)$ about its average value $\langle\rho(\mathbf{x})\rangle$, writing $\rho(x) = \langle\rho(\mathbf{x})\rangle + \delta\rho(x)$. The interaction can then be written

$$\begin{aligned} H_I &= -\frac{g}{2}\int_{\mathbf{x}}(\langle\rho(\mathbf{x})\rangle + \delta\rho(x))^2 \\ &= -\frac{g}{2}\int_{\mathbf{x}}\Big[\langle\rho(\mathbf{x})\rangle^2 + 2\langle\rho(\mathbf{x})\rangle\delta\rho(x)\Big] + O(\delta\rho(x)^2) \end{aligned} \tag{13.151}$$

  If we neglect the term second order in the fluctuations, then resubstitute $\delta\rho(x) = \rho(x) - \langle\rho(\mathbf{x})\rangle$, we obtain

$$H_I \approx -\frac{g}{2}\int_{\mathbf{x}}\Big[2\langle\rho(\mathbf{x})\rangle\rho(x) - \langle\rho(\mathbf{x})\rangle^2\Big] = \int_{\mathbf{x}}\Big[\rho(x)\phi(\mathbf{x}) + \frac{\phi(\mathbf{x})^2}{2g}\Big] \tag{13.152}$$

  where we have replaced $-g\langle\rho(\mathbf{x})\rangle = \phi(\mathbf{x})$. This approximate mean-field Hamiltonian (13.152) resembles the result of the Hubbard Stratonovich transformation (13.149)

With care, this kind of reasoning can be extended to a whole host of interactions between various kinds of charge, spin, current densities, including both non-local interactions and repulsive interactions. For example, in the Hubbard and Anderson models, the interaction can be written as an attractive interaction in the magnetic channel of the form that is factorized as follows:

$$-\frac{U}{2}(n_\uparrow - n_\downarrow)^2 \to (n_\uparrow - n_\downarrow)M + \frac{M^2}{2U} \tag{13.153}$$

corresponding to electrons exchanging fluctuations of the magnetic Weiss field M. The coupling between the field M and the electrons can sometimes stabilize a broken symmetry state where M develops an expectation value - leading to a magnet. The Hubbard Stratonovich transformation can also be applied to complex fields, permitting the following factorization

$$H_I = -gA^\dagger A \to \bar A\Delta + \bar\Delta A + \frac{\bar\Delta\Delta}{g} \tag{13.154}$$

where Δ is a complex field. Notice how we have switched $A^\dagger \to \bar A$ to emphasize that the replacement is only exact *under the path integral* (or alternatively, if you wish to switch to operators, under the time-ordering operator). This kind of interaction occurs in a BCS superconductor, where the pairing interaction

$$H_I = -g\sum_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}c_{-\mathbf{k}'\downarrow}c_{\mathbf{k}'\uparrow} = -g\overbrace{\sum_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}}^{A^\dagger}\overbrace{\sum_{\mathbf{k}} c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}}^{A}.$$

In this case, *under the path integral* the interaction can be rewritten in terms of electrons moving in a fluctuating pair field

$$H_I \to \bar\Delta\sum_{\mathbf{k}} c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} + \sum_{\mathbf{k}}\bar c_{\mathbf{k}\uparrow}\bar c_{-\mathbf{k}\downarrow}\Delta + \frac{\bar\Delta\Delta}{g}$$

Once superconductivity develops, Δ develops an expectation value, playing the role of an order parameter.

13.5.2 Detailed derivation

Let us examine the above procedure in detail. To be concrete, consider an attractive interation of the form $H_I = -g\sum_j A^\dagger{}_j A_j$, where A_j represents an electron bilinear (such as the pair density or spin density of an x-y spin). Consider a fermion path integral on a lattice with interactions $H_I = -g\sum_j A_j{}^\dagger A_j$,

$$Z = \int \mathcal{D}[\bar{c}, c] \exp\left[-\int_0^\beta d\tau \bar{c}(\partial_\tau + \underline{h})c - g\sum_j \bar{A}_j A_j\right], \tag{13.155}$$

where inside the path integral, we have replaced $A^\dagger \to \bar{A}$. The next step is to introduce a "white noise" variable, α_j described by the path integral

$$Z_\alpha = \int \mathcal{D}[\bar{\alpha}, \alpha] \exp\Big[-\sum_j \int_0^\beta d\tau \frac{\bar{\alpha}_j \alpha_j}{g}\Big]. \tag{13.156}$$

The weight function

$$\exp\left[-\sum_j \int_0^\beta d\tau \frac{\bar{\alpha}_j \alpha_j}{g}\right]$$

is a Gaussian distribution function for a white noise field with correlation function [2]

$$\langle \bar{\alpha}_i(\tau)\alpha_j(\tau')\rangle = g\delta_{ij}\delta(\tau - \tau'). \tag{13.157}$$

Now the product of these two path integrals

$$Z \times Z_\alpha = \int \mathcal{D}[\bar{c}, c] \int \mathcal{D}[\bar{\alpha}, \alpha] \exp\left[-\int_0^\beta d\tau \bar{c}(\partial_\tau + \underline{h})c - \sum_j \overbrace{\left(-g\bar{A}_j A_j + \frac{\bar{\alpha}_j \alpha_j}{g}\right)}^{H_I'(j)}\right], \tag{13.158}$$

describes two independent systems. As written, the "α" integrals are on the inside of the path so that for all configurations of the $\alpha_j(\tau)$ field explored in the inner α integral, the space-time configuration

[2] To show this, it is helpful to consider the generating functional

$$\Lambda[\bar{j}, j] = \int \mathcal{D}[\bar{\alpha}, \alpha] \exp\Big[-\sum_r \int_0^\beta d\tau \Big(\frac{\bar{\alpha}_r \alpha_r}{g} - \bar{j}_r \alpha_r - \bar{\alpha}_r j_r\Big)\Big]$$

By changing variables, $\alpha_r \to \alpha_r + g j_r$, we can absorb the terms linear in j, to obtain

$$\Lambda[\bar{j}, j] = \exp\Big[g\sum_r \int_0^\beta d\tau (\bar{j}_r(\tau) j_r(\tau))\Big]$$

Differentiating this with respect to $j_r(\tau)$, we find that

$$\frac{\partial^2 \ln\Lambda[j, \bar{j}]}{\partial \bar{j}_r(\tau)\partial j_{r'}(\tau')}\Big|_{j,\bar{j}=0} = \langle \alpha_r(\tau)\bar{\alpha}_{r'}(\tau')\rangle = g\delta_{rr'}\delta(\tau - \tau')$$

of the $A_j(\tau)$ set by the outer integral are frozen and can hence be regarded as "constants", fixed at each point in space time. This permits us to define a new variable

$$\Delta_j(\tau) = \alpha_j(\tau) - gA_j(\tau),$$

and its corresponding conjugate $\bar{\Delta}_j = \bar{\alpha}_j - g\bar{A}_j$. Formally this is just a shift in the integration variable, so the measure is unchanged and we can write $\mathcal{D}[\bar{\Delta}, \Delta] = \mathcal{D}[\bar{\alpha}, \alpha]$. The transformed interaction becomes

$$\begin{aligned} H_I' &= \sum_j \left\{-g\bar{A}_j A_j \frac{(\bar{\Delta}_j + g\bar{A}_j)(\Delta_j + gA_j)}{g}\right\} \\ &= \sum_j \left\{\bar{A}_j\,\Delta_j + \bar{\Delta}_j A_j + \frac{\bar{\Delta}_j \Delta_j}{g}\right\}. \end{aligned} \tag{13.159}$$

In this way, we arrive at a transformed interaction in which new variable Δ_j is linearly coupled to the electron operator A_j. If we now re-invert the order of integration inside the path integral (13.158), we obtain

$$\begin{aligned} Z &= \int \mathcal{D}[\bar{\Delta}, \Delta] \exp\left[-\sum_j \int_0^\beta d\tau \frac{\bar{\Delta}_j \Delta_j}{g}\right] \int \mathcal{D}[\bar{c}, c] e^{-\tilde{S}} \\ \tilde{S} &= \int_0^\beta d\tau \left(\bar{c}\partial_\tau c + H_E[\bar{\Delta}, \Delta]\right) \end{aligned} \tag{13.160}$$

where

$$H_E[\bar{\Delta}, \Delta] = \bar{c}\underline{h}c + \sum_j \left\{\bar{A}_j \Delta_j + \bar{\Delta}_j A_j\right\} \tag{13.161}$$

represents the action for electrons moving in the fluctuating field Δ_j. Notice that since A and $\bar{A}$ represent fermion bilinear terms, that *H_E is itself a bilinear Hamiltonian.*

These noisy fluctuations mediate the interaction between the fermions, much as an exchange boson mediates interactions in the vacuum. More schematically,

$$Z = \sum_{\{\Delta\}} \exp\left(-\sum_j \int d\tau \frac{|\Delta_j|^2}{g}\right) \times \Big[\text{ Path integral of fermions moving in field } \Delta\ \Big] \tag{13.162}$$

where the summation represents a sum over all possible configurations $\{\Delta\}$ of the auxiliary field Δ. The transformed field

$$\Delta_j = \alpha_j - gA_j$$

is a combination of a white noise field α_j and the physical field $-gA_j$, so its fluctuations now acquire the correlations associated with the electron fluid. Indeed, when the associated variable A is prone to

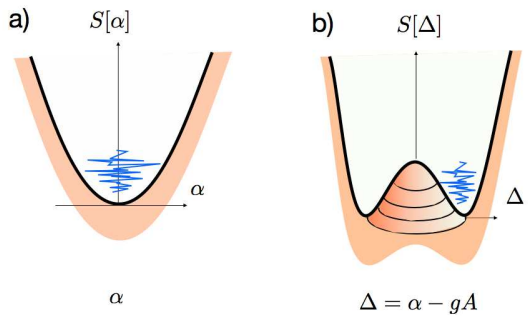


Figure 13.5: (a) Action for initial white noise variable α. (b) Action for shifted variable Δ is shifted off-centre when the related quantity A has a predisposition towards developing an expectation value.

the development of a broken-symmetry expectation value, the distribution function for Δ becomes concentrated around a non-zero value (Fig. 13.5). We call Δ_j a "Weiss field" after Weiss, who first introduced such a field in the context of magnetism.

13.5.3 Integrating out the fermions.

Since the fermionic action inside the path integral is actually Gaussian, we can formerly integrate out the fermions as follows

$$e^{-S_\phi[\bar\Delta,\Delta]} = \int \mathcal{D}[\bar c, c]e^{-\hat S} = \det[\partial_\tau + \underline{h}_E[\bar\Delta,\Delta]] \tag{13.163}$$

where $\underline{h}_E$ is the matrix representation of H_E. The Full path integral may thus be written

$$Z = \int \mathcal{D}[\bar\Delta,\Delta]e^{-S_E[\bar\Delta,\Delta]}$$

where

$$\begin{aligned} S_E[\bar\Delta,\Delta] &= \sum_j \int d\tau \frac{\bar\Delta_j\Delta_j}{g} - \ln\det[\partial_\tau + \underline{h}_E[\bar\Delta,\Delta]] \\ &= \sum_j \int d\tau \frac{\bar\Delta_j\Delta_j}{g} - \mathrm{Trln}[\partial_\tau + \underline{h}_E[\bar\Delta,\Delta]] \end{aligned} \tag{13.164}$$

where we have made the replacement $\ln\det \to \mathrm{Tr}\det$. This quantity is called the "effective action" of the field Δ. The additional fermionic contribution to this action can profoundly change the distribution of the field Δ. For example, if S_E develops a minima away around $\Delta = \Delta_o \neq 0$, the $\Delta = -A/g$

will acquire a "vacuum expectation value". This makes the Hubbard Stratonovich transformation an invaluable tool for studying the development of broken symmetry in interacting Fermi systems.

13.5.4 Generalizations to real variables and repulsive interactions

The method outlined in the previous section can also be applied to real fields. If we have a real Hamiltonian we can introduce a real white noise field as follows

$$H_I = -\frac{g}{2}\sum_j A_j^2 \to \sum_j \left\{-\frac{g}{2}A_j^2 + \frac{q_j^2}{2g}\right\} \tag{13.165}$$

and then by redefining $q_j = Q_j + gA_j$, one obtains

$$-\frac{g}{2}\sum_j A_j^2 \to \sum_j \left\{Q_jA_j + \frac{Q_j^2}{g}\right\} \tag{13.166}$$

For example, we can use the Hubbard Stratonovich transformation to replace an attractive interaction between fermions by a white noise potential with variance g:

$$H_I = -\frac{g}{2}\sum_j (n_j)^2 \to \sum_{j\sigma} V_j n_j + \frac{V_j^2}{2g}$$

where $n_j = n_{j\uparrow} + n_{j\downarrow}$.

But what about repulsive interactions? These require a little more care, because we can't just change the sign of g in (13.166) for the integral over the white noise fields will no longer be convergent. Instead, after introducing the dummy white noise fields as before,

$$H_I = \frac{g}{2}A_j^2 \to \sum_j \left\{\frac{g}{2}A_j^2 + \frac{q_j^2}{2g}\right\}, \tag{13.167}$$

to absorb the interaction, we shift each variable in the path integral $q_j(\tau)$ by an imaginary amount, $q_j(\tau) = Q_j(\tau) + igA_j(\tau)$, to obtain [3]

$$\frac{g}{2}\sum_j A_j^2 \to \sum_j \left\{iQ_jA_j + \frac{Q_j^2}{2g}\right\} \tag{13.168}$$

[3] One might be worried about the legitimacy of shifting a real field by an imaginary quantity. However, just as the integral

$$\int_{-\infty}^{\infty} dQe^{-Q^2/2} = \int_{-\infty+iA}^{\infty+iA} dQe^{-Q^2/2} =$$

is unaffected by a constant shift of the variable Q by an imaginary amount, $Q \to Q + iA$ axis, a multi-variable path integral

$$\int D[Q]e^{-\int d\tau Q(\tau)^2/2}$$

is similarly unaffected by shifting the integration variable $Q(\tau)$ by an amount $iA(\tau)$, $Q(\tau) \to Q(\tau) + iA(\tau)$.

Note finally, that if one replaces $Q_j = -i\bar{Q}_j$, this takes the form

$$\frac{g}{2}\sum A_j^2 \to \sum_j \left\{ \bar{Q}_j A_j - \frac{\bar{Q}_j^2}{2g} \right\} \tag{13.169}$$

Which first sight, looks like the generalization of (13.166) to negative g excepting now, the integrals over the each $Q_j(\tau)$ traverse the imaginary, rather than the real axis.

Example 13.6: Using the Hubbard Stratonovich transformation, show that the Coulomb interaction can be decoupled in terms of a fluctuating potential as follows:

$$H_I = \frac{1}{2}\int_{\mathbf{x},\,\mathbf{x}'} \rho(\mathbf{x})\rho(\mathbf{x}')\frac{e^2}{4\pi\epsilon_0|\mathbf{x}-\mathbf{x}'|} \to \int_{\mathbf{x}} \left[e\rho(\mathbf{x})\phi(\mathbf{x}) - \epsilon_0\frac{(\nabla\phi)^2}{2} \right] \tag{13.170}$$

What is the interpretation of the new term, quadratic in the potential field (and why is the sign negative)?

Solution: Because of the non-local nature of the Coulomb interaction, it is more transparent to make this transformation in momentum space. Writing

$$\rho(x) = \int_{\mathbf{q}} \rho_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}}, \qquad \frac{1}{\epsilon_0|\mathbf{x}-\mathbf{x}'|} = \int_{\mathbf{q}} \frac{1}{\epsilon_0 q^2} e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')} \tag{13.171}$$

where $\int_{\mathbf{q}} \equiv \int \frac{d^3q}{(2\pi)^3}$, the interaction becomes

$$H_I = \frac{1}{2}\int_{\mathbf{q}} \frac{(e\rho_{\mathbf{q}})(e\rho_{-\mathbf{q}})}{\epsilon_0 q^2}$$

We now add in a dummy white noise term,

$$H_I \to H_I' = \frac{1}{2}\int_{\mathbf{q}} \left[\frac{(e\rho_{\mathbf{q}})(e\rho_{-\mathbf{q}})}{\epsilon_0 q^2} - \epsilon_0 q^2 \phi_{\mathbf{q}}\phi_{-\mathbf{q}} \right],$$

with the understanding that in the path integral, the $\phi_{\mathbf{q}}$ field is to be integrated along the imaginary axis $\phi_{\mathbf{q}} = i\bar{\phi}_{\mathbf{q}}$. Now if we shift $\phi_{\mathbf{q}} \to \phi_{\mathbf{q}} - \frac{e\rho_{\mathbf{q}}}{\epsilon_0 q^2}$, we obtain

$$H_I' = \int_{\mathbf{q}} \left[(e\rho_{\mathbf{q}})\phi_{-\mathbf{q}} - \frac{\epsilon_0}{2} q^2 \phi_{\mathbf{q}}\phi_{-\mathbf{q}} \right]$$

Finally, Fourier transforming back into real space, ($q^2 \to -\nabla^2$) we obtain

$$H_I' = \int_{\mathbf{x}} \left[e\rho(x)\phi(x) + \frac{\epsilon_0}{2}\phi\nabla^2\phi \right] \tag{13.172}$$

Integrating the last term by parts gives

$$H_I' = \int_{\mathbf{x}} \left[e\rho(x)\phi(x) \overbrace{-\frac{\epsilon_0}{2}(\nabla\phi)^2}^{-\epsilon_0 E^2/2} \right] \tag{13.173}$$

We can identify the last term in this expression as $-\epsilon_0 E^2/2$, which is the electrostatic contribution to the action. The minus sign can be traced back to the fact that inside the electromagnetic (Maxwell) action

$$S_{EM} = \int d^3x d\tau \left[\frac{B^2}{2\mu_0} - \frac{\epsilon_0 E^2}{2} \right] \tag{13.174}$$

the electrostatic contribution to the action enters with the opposite sign to the magnetic part. The complete path integral for interacting electrons in this representation is then

$$Z = \int \mathcal{D}[\bar{\psi},\psi,\phi] \exp\left[-\int_0^\beta d\tau \int d^3x \left(\bar{\psi}(-\frac{1}{2m}\nabla^2 + e\phi(x) - \mu)\psi - \frac{\epsilon_0}{2}(\nabla\phi)^2 \right) \right].$$

Thus by carrying out a Hubbard Stratonovich transformation, the action becomes local. This formulation is ideal for the development of RPA approximations to the electron gas, while mean-field solutions of this path integral can be used to explore the formation of Wigner crystals.

13.6 Example: Magnetism in the Hubbard model.

To illustrate the Hubbard Stratonovich transformation, we now examine its application to the treatment of magnetism in the Hubbard model. Without spin, all matter would be magnetically inert (neither diamagnetic nor paramagnetic). Quantum mechanics provides an explanation of magnetism as a consequence of the orientational ordering of electron spins. This connection between magnetism and spin is one of the huge accomplishments of quantum mechanics.

13.6.1 Development of the theory of Itinerant Magnetism

Before our example, let me make a few remarks about the development of the theory of magnetism [14, 15]. A century ago, the ferro-magnetism of simple metals, such as iron, cobalt or nickel was an unsolved mystery. In 1906 the French physicist, Pierre Weiss working at ETH, Zurich, discovered that if you look at an ferromagnet on a small enough scale, it consists of magnetic domains. This led him to propose the first "mean-field theory", introducing the concept concept of an emergent "molecular" contribution to the effective internal magnetic field[16, 17]

$$\mathbf{H}_E = \mathbf{H} + \overbrace{I\mathbf{M}}^{\text{molecular Weiss field}} . \tag{13.175}$$

But the origin of the Weiss field was unknown. Worst, it quickly became clear that magnetism can't be understood using classical mechanics: indeed, according to the "Bohr-van Leeuwen theorem", independently proven by Neils Bohr and Hendrika van Leeuwen[18, 19] a fluid of (spinless) classical electrons *in thermal equilibrium* has zero magnetization, [4] even in a field[20].

[4] The Bohr-van Leeuwen theorem follows simply from the fact that the classical partition function of a gas of interacting particles can be transformed to show it is entirely independent of the applied field. The classical partition function is

This mystery was resolved by quantum mechanics and the discovery of "spin". In 1928, Werner Heisenberg, working at Leipzig made the critical link between magnetization and electron spin polarization; he also identified the Coulomb exchange interaction as the driving force for ferromagnetism [21] and the origin of the mysterious "I" in Weiss' theory. In the 1930's Edmund Stoner at Leeds University and John Slater at Harvard University developed the basis for an itinerant theory of ferromagnetism in metals[22, 23, 24]. A key idea here, is that strong interactions drive a metal to become unstable towards the development of a spontaneous spin polarization. In the simplest case, a ferromagnet develops, but later Albert Overhauser, working at Ford Labs in the early 1960s, showed the instability can also occur at a finite wavevector $\mathbf{Q}$ to form a *spin density wave*[25], as in the case of metallic chromium. This instability occurs when the product of the electron interaction I and "bare" magnetic susceptibility of the non-interacting electron gas at this wavevector $\chi_0(\mathbf{Q})$ reaches unity

$$I_{\mathbf{Q}}\chi_0(\mathbf{Q}) = 1, \qquad \textbf{(Stoner criterion)}.$$

Later in the 1960s, Junjiro Kanamori[26] at Osaka University and John Hubbard[27] in Harwell, England reformulated the theory of magnetism using the model we now call the Hubbard model. Sebastian Doniach and Stanley Engelsberg[28] at Imperial College London, and Norman Berk and Robert Schrieffer[29] at the University of Pennsylvannia, refined this work, demonstrating that quantum fluctuations of the magnetization play a crucial role: these fluctuations act to suppress the magnetization and become particularly strong near the point of instability or critical point. It is only recently that physicists have been able to experimentally examine such quantum critical points.

Itinerant magnetism is only one part of the story of magnetism, for in magnetic materials where the electrons are localized, the magnetization derives from "localized magnetic moments". High performance neodynium-iron alloy magnets derive their strength from localized moments on at the neodynium sites. Many of the most fascinating systems of current study, such as the high temperature cuprate and iron-based superconductors appear to lie in a murky region between "intineracy" and "localization", where electrons are on the brink of localization. This is a topic we shall return to chapter 15.

written

$$Z = \int \prod_{i=1,N} d^3p_i d^3x_i e^{-\beta H} \tag{13.176}$$

where

$$H[\mathbf{p},\mathbf{x}] = \sum_i \frac{(\mathbf{p}_i - e\mathbf{A}(\mathbf{x}_i))^2}{2m} + \sum_{i<j} U(\mathbf{x}_i - \mathbf{x}_j) + e\phi(\mathbf{x}_i)$$

where all the magnetic field dependence lies in the vector potential term, given by $\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{x}$ in the Landau gauge. However, one can always make the change of variable $\mathbf{p}' = \mathbf{p} + e\mathbf{A}(\mathbf{x}), \mathbf{x}' = \mathbf{x}$, for which the Jacobian is unity, completely absorbing all dependence on the external magnetic field. The equilibrium magnetization, $\mathbf{M} = -\mathbf{T}\delta\mathbf{lnZ}/\delta\mathbf{B}(\mathbf{x}) = \mathbf{0}$ is therefore zero. This also implies that the isothermal magnetic susceptibility of a classical plasma is zero. Note however that a classical electron gas does have a diamagnetic response when a field is applied adiabatically, rather than isothermally.

13.6.2 Path integral formulation of the Hubbard Model

We encountered the Hubbard model in Chapter 5. It consists of a single band of electrons moving on a tight-binding lattice, with a localized interaction of strength U, described by the Hamiltonian

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U\sum_j n_{j\uparrow}n_{j\downarrow}. \tag{13.177}$$

where

$$c_{\mathbf{k}\sigma} = \frac{1}{\sqrt{N_s}}\sum c^\dagger{}_{j\sigma} e^{i\mathbf{k}\cdot\mathbf{r}_j}$$

creates an electron of wavevector $\mathbf{k}$ with energy $\epsilon_{\mathbf{k}}$. To explore magnetism in this model we rewrite the interaction term in terms of the spin operators as follows

$$Un_{j\uparrow}n_{j\downarrow} = -\frac{U}{2}(n_{j\uparrow} - n_{j\downarrow})^2 + \frac{U}{2}(n_{j\uparrow} + n_{j\downarrow}). \tag{13.178}$$

where we have used the fact that $n^2_{j\uparrow} = n_{j\uparrow}$. Now as written, the above decoupling emphasizes the magnetic fluctuations along the $z-$ axis. Indded, we might have made the decoupling around any spin quantization axis, and since we are interested in keeping track of magnetic fluctuations along all axes it makes sense to average over all three directions, writing the decoupling as

$$Un_{j\uparrow}n_{j\downarrow} = -\frac{U}{6}\Big(\boldsymbol{\sigma}_j\Big)^2 + \frac{U}{2}(n_{j\uparrow} + n_{j\downarrow}), \tag{13.179}$$

where we have introduced the notation $\boldsymbol{\sigma}_j = (c^\dagger{}_{j\alpha}\boldsymbol{\sigma}_{\alpha\beta}c_{j\beta})$ for the magnetization at site j. The second term in this expression can be absorbed into a redefinition of the chemical potential, by writing $\mu = \mu' + U/2$. The minus sign in this interaction manifestly displays magnetic exchange effect of the Coulomb interaction, whereby a repulsion between charges leads to an *attraction between spins*.

We now formulate the problem as a path integral

$$\begin{aligned} Z &= \int \mathcal{D}[c]e^{-S} \\ S &= \int_0^\beta d\tau\Big[\sum_{\mathbf{k},\sigma}\bar{c}_{\mathbf{k}\sigma}(\partial_\tau + \epsilon_{\mathbf{k}})c_{\mathbf{k}\sigma} - \frac{I}{2}\sum_j(\boldsymbol{\sigma}_j)^2\Big], \qquad (I = U/3), \end{aligned} \tag{13.180}$$

where we have introduced the coupling constant $I = U/3$. At this point, we carry out a Hubbard Stratonovich transformation. Adding a white noise field m_j into the action, so that

$$-\frac{I}{2}\sum_j(\boldsymbol{\sigma}_j)^2 \to -\frac{I}{2}\sum_j(\boldsymbol{\sigma}_j)^2 + \int_0^\beta d\tau\sum_j\frac{\mathbf{m}_j^2}{2I}, \tag{13.181}$$

and then shifting $\mathbf{m}_j = \mathbf{M}_j - I\boldsymbol{\sigma}_j$, we obtain

$$-\frac{I}{2}(\boldsymbol{\sigma}_j)^2 \to -\mathbf{M}_j(\tau)\cdot\boldsymbol{\sigma}_j + \frac{\mathbf{M}_j(\tau)^2}{2I}, \tag{13.182}$$

where $\mathbf{M}_j(\tau)$ is a fluctuating Weiss field. We have chosen the sign of the first term to reflect the role of the Weiss field as "effective magnetic field". The transformed partition function

$$\begin{aligned} Z &= \int \mathcal{D}[\mathbf{M},\bar{c},c]e^{-S[\bar{c},c,\mathbf{M}]}, \\ S[\bar{c},c,\mathbf{M}] &= \int_0^\beta d\tau\left(\sum_{\mathbf{k},\sigma}\bar{c}_{\mathbf{k}\sigma}(\partial_\tau+\epsilon_{\mathbf{k}})c_{\mathbf{k}\sigma}+\sum_j\Big[-\mathbf{M}_j\cdot\boldsymbol{\sigma}_j+\frac{\mathbf{M}_j{}^2}{2I}\Big]\right), \end{aligned} \tag{13.183}$$

describes electrons moving through a lattice of fluctuating magnetization. We can emphasize this interpretation by moving the magnetization integral to the outside, writing

$$Z=\int\mathcal{D}[\mathbf{M}]e^{-S_E[\mathbf{M}]} \tag{13.184}$$

where the effective action

$$e^{-S_E[\mathbf{M}]}=\int\mathcal{D}[\bar{c},c]e^{-S[\bar{c},c,\mathbf{M}]} \tag{13.185}$$

describes the action associated with a particular space-time configuration $\{\mathbf{M}_j(\tau)\}$ of the magnetization. Since the exponential $S[\bar{c},c,\mathbf{M}]$ in (13.185) is a quadratic function of fermion fields, the integral is Gaussian and can be evaluted in closed form. To carry out the integral, it is convenient to Fourier transform the fields, writing $c_{j\sigma}=\frac{1}{\sqrt{N_s}}\sum_{\mathbf{k}}c_{\mathbf{k}\sigma}e^{i\mathbf{k}\cdot\mathbf{x}_j}$, so that

$$\sum_{j\sigma}\mathbf{M}_j\cdot\boldsymbol{\sigma}_j=\sum_{j\sigma}\mathbf{M}_j\cdot(\bar{c}_{j\alpha}\boldsymbol{\sigma}_{\alpha\beta}c_{j\beta})=\sum_{\mathbf{k},\mathbf{k}',\sigma}\bar{c}_{\mathbf{k}'\alpha}(\mathbf{M}_{\mathbf{k}'-\mathbf{k}}\cdot\boldsymbol{\sigma}_{\alpha\beta})c_{\mathbf{k}\beta} \tag{13.186}$$

where $\mathbf{M}_{\mathbf{q}}=\frac{1}{N_s}\sum_j\mathbf{M}_je^{-i\mathbf{q}\cdot\mathbf{R}_j}$ is the Fourier transform of the magnetization. The effective action can be written in the compact form

$$e^{-S_E[\mathbf{M}]}=\int\mathcal{D}[\bar{c},c]\exp\left[-\int_0^\beta d\tau\left(\bar{c}(\partial_\tau+\underline{h}_E[\mathbf{M}])c+\sum_j\frac{\mathbf{M}_j^2}{2I}\right)\right] \tag{13.187}$$

where,

$$[\underline{h}_E]_{\mathbf{k}',\mathbf{k}}=\epsilon_{\mathbf{k}}\delta_{\mathbf{k},\mathbf{k}'}-\mathbf{M}_{\mathbf{k}'-\mathbf{k}}(\tau)\cdot\boldsymbol{\sigma} \tag{13.188}$$

describes the effective Hamiltonian for the electrons moving in the (time dependent) magnetization field. Carrying out the Gaussian integral over $\bar{c}$ and c using (13.133) then gives

$$e^{-S_E[\mathbf{M}]}=\mathrm{Det}\Big[\partial_\tau+h_E[\mathbf{M}]\Big]\exp\left[-\sum_j\int_0^\beta d\tau\frac{\mathbf{M}_j^2}{2I}\right], \tag{13.189}$$

or more explicitly,

$$S_E[\mathbf{M}]=\overbrace{-\mathrm{Tr}\ln\left[(\partial_\tau+\epsilon_{\mathbf{k}})\delta_{\mathbf{k}',\mathbf{k}}-\mathbf{M}_{\mathbf{k}'-\mathbf{k}}\cdot\boldsymbol{\sigma}\right]}^{-\ln\mathrm{Det}[\partial_\tau+h_E]}+\sum_j\int_0^\beta d\tau\frac{\mathbf{M}_j^2}{2I}. \tag{13.190}$$

Note that

- In general, we can only evaluate S_E analytically for simple static configurations of $\mathbf{M}_j(\tau)=\mathbf{M}_j$. These provide the basis for mean-field theories.
- The factor $e^{-S_E[M]}$ in (13.189) resembles a Boltzmann distribution in classical statistical mechanics. However, in striking distinction with its classical counterpart, in certain non-uniform configurations of the magnetization the weigth function $e^{-S_E[M]}$ acquires negative values. These configurations are in many ways, the most interesting configurations of the path integral, and when they proliferate, standard Metropolis Monte Carlo approaches become exceedingly inaccurate. This is "the minus sign problem" of many body physics - one of the major unsolved problems of numerical Many Body physics.

It is also useful to cast the effective action in terms of Feynman diagrams. To do this, we first rewrite the magnetization in terms of its Matsubara Fourier modes,

$$\mathbf{M}_q\equiv\mathbf{M}_{\mathbf{q}}(i\nu_n)=\frac{1}{\beta}\int_0^\beta d\tau\,\mathbf{M}_{\mathbf{q}}(\tau)e^{i\nu_n\tau} \tag{13.191}$$

In Fourier space, we replace $\partial_\tau\to-i\omega_n$ in the Fermionic Determinant of (13.190) to obtain

$$S_E[\mathbf{M}]=-\mathrm{Tr}\ln\left[(-i\omega_n+\epsilon_{\mathbf{k}})\delta_{k,k'}-\mathbf{M}_{k-k'}\cdot\boldsymbol{\sigma}\right]+N_s\beta\sum_q\frac{|\mathbf{M}_q|^2}{2I}. \tag{13.192}$$

We can factor out $(-i\omega+\epsilon_{\mathbf{k}})$ inside the logarithm, which permits us to split it into two terms,

$$\begin{aligned} S_E[\mathbf{M}] &= -\mathrm{Tr}\ln\Big[(-i\omega_n+\epsilon_{\mathbf{k}})(1+(i\omega_n-\epsilon_{\mathbf{k}})^{-1}\mathbf{M}_{k-k'}\cdot\boldsymbol{\sigma})\Big]+N_s\beta\sum_q\frac{|\mathbf{M}_q|^2}{2I} \\ &= -\mathrm{Tr}\ln\left[(-i\omega_n+\epsilon_{\mathbf{k}})\right]-\overbrace{\mathrm{Tr}\ln\left[1-G_0(k)V_{k,k'}\right]}^{\mathrm{Tr}\ln(1-G_0V)}+N_s\beta\sum_q\frac{|\mathbf{M}_q|^2}{2I}. \end{aligned} \tag{13.193}$$

where

$$G_0(k)=(i\omega_n-\epsilon_{\mathbf{k}})^{-1},\ V_{k,k'}=-\mathbf{M}_{k-k'}\cdot\boldsymbol{\sigma}. \tag{13.194}$$

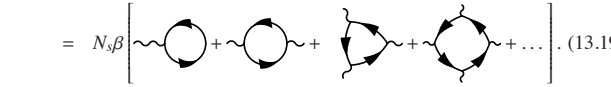
Here we have used the identity $\mathrm{Tr}[\ln(AB)]=\mathrm{Tr}\ln A+\mathrm{Tr}\ln B$ to seperate the terms inside the logarithm. Normalized with respect to the volume of space time, The first term in (13.193) can be

normalized to give the free energy density fo the non-interacting system

$$\mathcal{F}_0 = \frac{S_0}{N_s\beta} = -\frac{1}{N_s\beta}\mathrm{Tr}\ln\left[(-i\omega_n + \epsilon_{\mathbf{k}})\right].$$

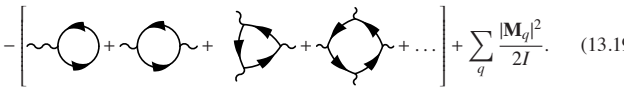
The second term is the change in the Free energy of the fermions due to the magnetization field: the overbrace shows how we can rewrite it in terms of the bare propagator $G_0 = (i\omega_n - \epsilon_{\mathbf{k}})^{-1}$ and the scattering potential $V_{k',k} = -\mathbf{M}_{k'-k}\cdot\boldsymbol{\sigma}$. This term can be reinterpreted as an infinite sum of Feynman diagrams, describing repeated scattering off the exchange field

$$\begin{aligned}\mathrm{Tr}\ln(1 - G_0V) &= \mathrm{Tr}[-G_0V - \frac{1}{2}(G_0V)^2 - \frac{1}{3}(G_0V)^3 + \dots] \\ &= N_s\beta\Bigg[\quad + \quad + \quad + \quad + \dots\Bigg].\end{aligned} \tag{13.195}$$



The pre-factor $N_s\beta$, the volume of space-time, is included because we are working in Fourier space, with the convention that all internal momentum and frequency sums are normalized with a measure $\frac{1}{N_s\beta}\sum_{\mathbf{k},i\omega_n}$. The effective free energy (per site) $\mathcal{F}_E[\mathbf{M}] = S_E/(N_s\beta)$ can then be written diagrammatically as

$$\mathcal{F}_E[\mathbf{M}] = \mathcal{F}_0 - \Bigg[\quad + \quad + \quad + \quad + \dots\Bigg] + \sum_q \frac{|\mathbf{M}_q|^2}{2I}. \tag{13.196}$$



13.6.3 Saddle point and the Mean field theory of magnetism

To explore broken symmetry solutions, we now make a saddle point approximation, approximating the partition function by its value at the saddle-point $\mathbf{M} = \mathbf{M}_0$

$$\boxed{Z = \int \mathcal{D}[M]e^{-S_E[\mathbf{M}]} \approx e^{-S_E[\mathbf{M}_0]}} \tag{13.197}$$

where

$$\left.\frac{\delta S_E[\mathbf{M}]}{\delta\mathbf{M}}\right|_{\mathbf{M}=\mathbf{M}^{(0)}} = 0. \tag{13.198}$$

Equations (13.197) and (13.198) contain the essence of mean-field theory and deserve some discussion. We discussed in Chapter 13 how a system develops a spontaneously broken symmetry when the Landau functional $F[M]$ develops a minimum at a non-zero value of the order parameter. A full-fledged calculation of this functional would involve calculating the full path-integral $Z[h]$ with a symmetry breaking field h in place, using a Legendre transformation to calculate $S[M] = S[h] - h.\delta S/\delta h$, ultimately taking h to zero the end of the calculation. The mean-field approach

approximates $S[\mathbf{M}] \approx S_E[\mathbf{M}]$. Such "saddle point" or "mean-field" solutions serve as the staging point to compute the fluctuations around the broken symmetry state. The ultimate consistency of any mean-field approximation depends on the fluctuations being small enough that they do not wash out the broken symmetry solution.

If we differentiate $S_E[\mathbf{M}]$ in (13.185), we see that the saddle point condition (13.198) implies

$$\frac{\delta S_E}{\delta\mathbf{M}_j} = = \frac{1}{e^{-S_E}}\int \mathcal{D}[\bar{c},c]\overbrace{\left(\frac{\mathbf{M}_j}{I} - \bar{c}_j\boldsymbol{\sigma}c_j\right)}^{\frac{\delta S[\bar{c},c,\mathbf{M}]}{\delta\mathbf{M}_j}}e^{-S[\bar{c},c,\mathbf{M}]} = \frac{\mathbf{M}_j}{I} - \langle c^\dagger{}_j\boldsymbol{\sigma}c_j\rangle\Big|_{h_E}. \tag{13.199}$$

where we have used (13.183) to calculate $\delta S[\bar{c},c,\mathbf{M}]/\delta\mathbf{M}_j$. In this way the saddle point condition (13.198) automatically satisfies the mean-field relation

$$\underbrace{\left.\frac{\delta S[\mathbf{M}]}{\delta\mathbf{M}_j}\right|_{\mathbf{M}=\mathbf{M}_0} = 0}_{\text{Saddle point condition}}, \quad \Longleftrightarrow \quad \underbrace{\mathbf{M}_j^{(0)} = I\,\langle c^\dagger{}_j\boldsymbol{\sigma}c_j\rangle\big|_{h_E[\mathbf{M}^{(0)}]}}_{\text{Mean field theory.}} \tag{13.200}$$

This makes life a lot easier: instead of labouring to impose the self-consistency condition on the right-hand side, we can simply generate mean-field solutions by minimizing the effective action. Generally, we're interested in a static saddle point, where $\mathbf{M}_j(\tau) = \mathbf{M}_j^{(0)}$, In this situation, the effective action is directly related to the mean-field partition function

$$e^{-S_E[\mathbf{M}^{(0)}]} = \mathrm{Tr}\left[e^{-\beta\hat{H}_{MF}}\right] \tag{13.201}$$

where

$$\hat{H}_{MF} = c^\dagger\underline{h}_E[\mathbf{M}^{(0)}]\,c + \sum_j\frac{(\mathbf{M}_j^{(0)})^2}{2I}, \tag{13.202}$$

is read off from the action in the path integral (13.187).

In a ferromagnet, the magnetization is uniform: for convenience we choose the spin-polarization along the z-axis, writing

$$\mathbf{M}_j^{(0)} = M\hat{\mathbf{z}}, \tag{13.203}$$

or in in Fourier space $\mathbf{M}_\mathbf{q} = M\delta_\mathbf{q}\,\hat{\mathbf{z}}$. In this case, the mean-field Hamiltonian is diagonal:

$$H_{MF} = \sum_{\mathbf{k}\sigma} c^\dagger{}_{\mathbf{k}\sigma}(\epsilon_\mathbf{k} - \sigma M)c_{\mathbf{k}\sigma} + N_s\frac{M^2}{2I} \tag{13.204}$$

since $M_q = M\delta_{q0}$. We see that when M is finite, the up and down Fermi surfaces are now exchange split by an amount $\Delta = 2M$. By carrying out the Gaussian integral over the Fermi fields, or substituting into (13.192) we can immediately write down the effective action as

$$S_E[M] = -\sum_{\mathbf{k},i\omega_n}\mathrm{Tr}\ln\left[\epsilon_\mathbf{k} - M\sigma_z - i\omega_n\right] + N_s\beta\frac{M^2}{2I} \tag{13.205}$$

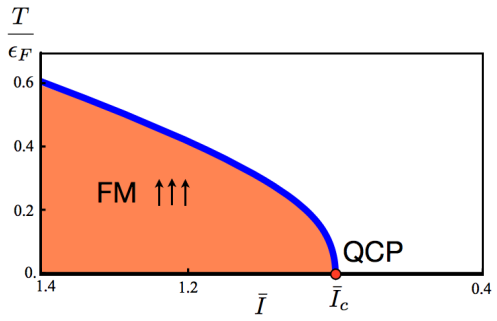


Figure 13.6: Phase diagram for 3D "Stoner model" computed using using (13.211) and (13.212). The horizontal axis is the coupling constant $\bar{I} = IN(0)$, where the critical value $\bar{I}_c = 1$.

The result of carrying out the Matsubara sum on this expression gives the well known form

$$\begin{aligned}\mathcal{F}_E[M] &= -\frac{1}{N_s\beta}\sum_{\mathbf{k},\sigma}\ln[1+e^{-\beta(\epsilon_{\mathbf{k}}-\sigma M)}] + \frac{M^2}{2I} \\ &= -\frac{T}{2}\int d\epsilon N(\epsilon)\sum_{\sigma}\ln[1+e^{-\beta(\epsilon-\sigma M)}] + \frac{M^2}{2I}, \end{aligned} \tag{13.206}$$

where $\mathcal{F}_E = S_E/(\beta N_s)$ is the Free energy per unit volume, and we have rewritten the momentum summation as an integral, over the density of states per site $N(\epsilon)$.

To find the stationary point of the action, we differentiate it with respect to M to get

$$-\frac{\partial \mathcal{F}_E[M]}{\partial M} = 0 = \frac{M}{I} - \overbrace{\frac{1}{2}\sum_{\sigma=\pm 1}\int d\epsilon N(\epsilon) f(\epsilon-\sigma M)\sigma}^{\langle\sigma^z\rangle} \tag{13.207}$$

or

$$M = \frac{I}{2}\sum_{\sigma=\pm 1}\int d\epsilon N(\epsilon) f(\epsilon-\sigma M)\sigma \tag{13.208}$$

which expresses the mean-field condition $M = I\langle\sigma^z\rangle$. We can obtain the second-order phase transition temperature T_c by letting $M \to 0^+$. Replacing $f(\epsilon - \sigma M) \to f(\epsilon) - \sigma M f'(\epsilon)$ gives

$$1 = \overbrace{I\int d\epsilon N(\epsilon)\left(-\frac{df}{d\epsilon}\right)\Big|_{T=T_c}}^{\chi_0(T_c)} = I\chi_0(T_c) \qquad \text{(Stoner Criterion)}$$

where we have identified bracketed term as the spin-susceptibility of the non-interacting gas at T_c. At a finite temperature the Stoner Criterion defines the Curie temperature T_c of the electron gas. In the ground-state at absolute zero, we can replace the derivative of the Fermi function by a delta function $-df/d\epsilon \to \delta(\epsilon)$ so the Stoner Criterion becomes

$$I_c N(0) = 1 \qquad \text{(Stoner Criterion } T = 0\text{)}$$

where $I = I_c$ is the critical value of the interaction I, beyond which the paramagnetic *ground-state* becomes unstable to magnetism, as shown in Fig (13.6). This is a *quantum phase transition*, driven not by thermal, but by quantum fluctuations.

Example 13.7: Calculate the magnetic phase boundary $Tc(I)$ for the 3D continuum Stoner model, where the density of states $N(\epsilon) = N(0)\sqrt{\frac{\epsilon+\mu}{\epsilon_F}}$, where ϵ_F is the Fermi temperature and $N(0)$ the density of states at the Fermi surface.

Solution: In three dimensions, the Stoner Criterion can be written

$$\begin{aligned} 1 &= IN(0)\int_0^\infty dE\sqrt{\frac{E}{\epsilon_F}}\frac{f(E-\mu)[1-f(E-\mu)]}{T_c} \\ &= I\sqrt{\frac{T_c}{2\epsilon_F}}\int_0^\infty dx\sqrt{x}\,\mathrm{sech}^2[x-\mu\beta_c/2] \end{aligned} \tag{13.209}$$

If we were interested in the problem at constant chemical potential, we could stop here, however if we wish to take account of the drift of the chemical potential at finite temperature, we need to impose the condition of constant particle density n_0,

$$\begin{aligned} n_0 &= N(0)\int_0^\infty dE\sqrt{\frac{E}{\epsilon_F}}f(E-\mu) \\ &= N(0)\epsilon_F\left(\frac{T_c}{\epsilon_F}\right)^{\frac{3}{2}}\int_0^\infty dx\sqrt{x}\frac{1}{e^{x-\mu\beta_c}+1}. \end{aligned} \tag{13.210}$$

At zero temperature, this gives $n_0 = \frac{2}{3}N(0)\epsilon_F$, so that

$$\frac{2}{3}N(0)\epsilon_F = N(0)\epsilon_F\left(\frac{T_c}{\epsilon_F}\right)^{\frac{3}{2}}\int_0^\infty dx\sqrt{x}\frac{1}{e^{x-\mu\beta_c}+1}.$$

enabling us to write T_c as a parametric function of $y = \mu\beta_c$

$$T_c(y) = \epsilon_F\left[\frac{3}{2}\int_0^\infty dx\sqrt{x}\frac{1}{e^{x-y}+1}\right]^{-2/3}. \tag{13.211}$$

Inserting (13.211) into (13.209) we can also write $\bar{I} = IN(0)$ as a parametric function of $y = \mu\beta_c$,

$$\bar{I}(y) = \frac{\left[\frac{3}{2}\int_0^\infty dx\sqrt{x}\frac{1}{e^{x-y}+1}\right]^{1/3}}{\frac{1}{\sqrt{2}}\int_0^\infty dx\sqrt{x}\,\mathrm{sech}^2[x-y/2]}. \tag{13.212}$$

Fig (13.6) shows the phase diagram computed using (13.211) and (13.212)

To finish this section, let us calculate the Landau expansion of the Free energy. If we make a binomial expansion of the logarithm in $S_E[M]$ in powers of M, we obtain

$$-\frac{T}{2}\sum_{\sigma}\ln[1+e^{-\beta(\epsilon-\sigma M)}] = -T\ln[1+e^{-\beta\epsilon}] + \sum_{r=1}^{\infty}\frac{M^{2r}}{(2r)!}\frac{d^{2r-1}f(\epsilon)}{d\epsilon^{2r-1}} \tag{13.213}$$

where odd powers of M vanish and $f(\epsilon)$ is the Fermi function. Thus

$$\mathcal{F}[M] = \mathcal{F}_0 + \sum_{r=1}^{\infty}\frac{M^{2r}}{(2r)!}\int d\epsilon N(\epsilon)\frac{d^{2r-1}f(\epsilon)}{d\epsilon^{2r-1}} + \frac{M^2}{2I}. \tag{13.214}$$

If we integrate in (13.214) by parts, we obtain

$$\mathcal{F}[M] = \mathcal{F}_0 - \sum_{r}\frac{M^{2r}}{(2r)!}\overbrace{\int d\epsilon\left(-\frac{df}{d\epsilon}\right)N^{(2r-2)}(\epsilon)}^{\overline{N^{(2r-2)}(0)}} + \frac{M^2}{2I}. \tag{13.215}$$

where $N^{(r)} = d^rN(\epsilon)/d\epsilon^r$ is the r-th derivative of the density of states and $\overline{N^{(r)}(0)}$ is its corresponding thermal average around the Fermi surface. If we take terms up to M^4, we obtain

$$\mathcal{F} = \mathcal{F}_0 + \frac{1}{2}M^2\left(\frac{1}{I} - \chi_0(T)\right) + \frac{M^4}{4!}\overline{(-N''(0))} + O(M^6) \tag{13.216}$$

where $\overline{(-N''(0))}$ denotes the thermal average average of the second derivative of the density of states around the Fermi energy. This is the Landau energy function predicted by the "Stoner theory" of itinerant ferromagnet. Note that

- The quartic coefficient in the Free energy is positive, only if $\overline{N''(0)} < 0$ is negative, i.e, if the density of states has a downward curvature. If this requirement is not met, the ferromagnetic phase transition becomes first order. Most transition metal ferromagnets, such as iron and cobalt, involve narrow bands in three dimensions with a large negative curvature of the density of states and the transition is second-order. However, in quasi-two dimensional systems where the density of states has mostly positive curvature, the ferromagnetic phase transition is expected to be first order.

- The mean-field parameters in the above action are likely to be modified by fluctuations. In our mean-field theory, an isotropic decoupling gave $I = U/3$, but had we chosen an Ising decoupling, just in the z direction, we would have obtained $I = U$, which is most likely an over-estimate of I. Mean-field theories can not in general give a very reliable indication of the absolute size of such parameters.

- There is a formal "large N limit" in which the above mean-field theory does become exact. If instead of the original model, we chose a multi-band (N-band) model, with the action

$$S = \int_0^{\beta}d\tau\left[\sum_{\mathbf{k},\lambda\sigma}\bar{c}_{\mathbf{k}\lambda\sigma}(\partial_\tau + \epsilon_{\mathbf{k}})c_{\mathbf{k}\sigma} - \frac{I}{2N}\sum_j\Big(\sum_{\lambda}\boldsymbol{\sigma}_\lambda(j)\Big)^2\right] \tag{13.217}$$

where the band index $\lambda \in [1, N]$. Here the interaction I can be regarded as a "Hund's" interaction between the different bands. For large N the action of this model grows extensively with N, and in this situation, the path integral becomes saturated by the saddle-point solution, so the mean-field theory becomes exact.

Example 13.8:

(a) Show from the Landau energy (13.216), that near the quantum critical point at $T = 0$, $I = I_c = 1/N(0)$, the magnetic moment is given by

$$M = \sqrt{\left(\frac{I-I_c}{II_c}\right)\frac{6}{-N''(0)}} \sim \sqrt{I-I_c}. \tag{13.218}$$

(b) By expanding the density of states in a power-series about the Fermi energy, show that the transition temperature predicted by (13.216) is

$$T_c = \sqrt{\frac{6}{\pi^2}\left(\frac{1}{I} - N(0)\right)\frac{1}{(-N''(0))}}.$$

Solution: (a) We begin by writing the Landau free energy as

$$\mathcal{F} = \frac{rM^2}{2} + \frac{uM^4}{4}$$

where $r = I^{-1} - \overline{N(0)}$, $u = \overline{-N''(0)}/6$. At zero temperature,

$$r = \left(\frac{1}{I} - \frac{1}{I_c}\right), \qquad u = \frac{-N''(0)}{6}$$

where $I_c = 1/N(0)$. Setting $\partial F/\partial M^2 = 0$, we obtain $rM + uM^3 = 0$, or

$$M = \sqrt{\frac{r}{u}} = \sqrt{\left(\frac{I-I_c}{II_c}\right)\frac{6}{-N''(0)}} \sim \sqrt{I-I_c}.$$

(b) Carrying out a Taylor expansion of the density of states,

$$\overline{N(0)} = \int d\epsilon\left(-\frac{df}{d\epsilon}\right)\left[N(0) + \epsilon N'(0) + \frac{\epsilon^2}{2}N''(0)\right] = N(0) + \frac{\pi^2T^2}{6}N''(0)$$

it follows that at a small finite temperature

$$r(T) = \left(\frac{1}{I} - \frac{1}{I_c} + \frac{\pi^2T^2}{6}(-N''(0))\right)$$

Setting $r(T_c) = 0$, it follows that

$$T_c = \sqrt{\frac{6}{\pi^2}\left(\frac{1}{I} - N(0)\right)\frac{1}{(-N''(0))}}.$$

13.6.4 Quantum fluctuations in the magnetization

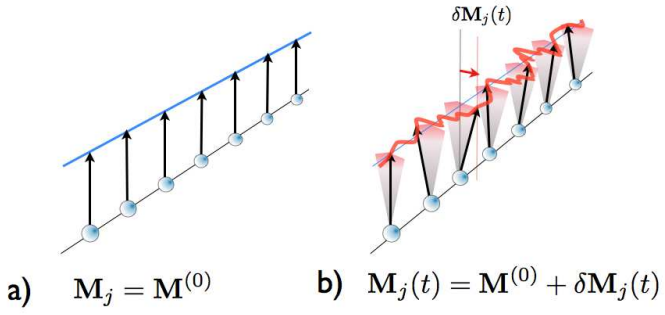


Figure 13.7: Illustrating (a) mean-field theory (b) fluctuations about mean-field theory.

The beauty of the saddle point approach, is that it allows one to go beyond the mean-field theory to examine the fluctuations in the order parameter. The basic idea is to expand the magnetization in fluctuations around the saddle point, writing

$$\mathbf{M}_j(\tau) = \mathbf{M}^{(0)} + \delta\mathbf{M}_j(\tau) \tag{13.219}$$

or in Fourier space

$$\mathbf{M}_q = \mathbf{M}^{(0)}\delta_{q=0} + \delta M_q, \qquad (q \equiv (\mathbf{q}, i\nu_n)) \tag{13.220}$$

Because the effective action is stationary with respect to variations in $\mathbf{M}$ at the saddle point, the leading order corrections to the effective action are quadratic in the fluctuations,

$$S_E[\mathbf{M}] = S_E[\mathbf{M}^{(0)}] + \frac{1}{2}\sum_q \frac{\delta^2 S}{\delta M^a_q \delta M^b_{-q}} \delta\mathbf{M}^a_q \delta\mathbf{M}^b_{-q} + O(\delta\mathbf{M}^3)$$

Notice that all linear terms in the fluctuations vanish by virtue of the fact that the mean-field action is stationary with respect to fluctuations. Provided the fluctuations are small compared to the order parameter, one can use the quadratic approximation to the effective action to examine the leading fluctuations of the magenization in the ferromagnetic state.

In a magnet these fluctuations take place against a *broken symmetry* background. The electrons scattering off the fluctuations are partially spin polarized and governed by the "renormalized" propagator, denoted by the double line

$$= \underline{G}(k) = (i\omega_n - \epsilon_{\mathbf{k}} - \sigma_z M)^{-1}.$$

where we have underlined $\underline{G}(k)$ to emphasize that it is a two-dimensional, albeit diagonal, matrix.

Let us now expand the effective action $S_E[\mathbf{M}]$ in (13.192) in the fluctuations by substituting $M_{k-k'} = M\delta_{k-k'} + \delta M_{k-k'}$ to obtain

$$\mathcal{F}_E[\mathbf{M}] = -\frac{1}{N_s\beta}\mathrm{Tr}\ln\left[-\underline{G}(k)^{-1}\delta_{k,k'} - \delta\mathbf{M}_{k-k'}\cdot\boldsymbol{\sigma}\right] + \sum_q \frac{|M\hat{\mathbf{z}}\delta_q + \delta\mathbf{M}_q|^2}{2I}. \tag{13.221}$$

If we now expand this expression in powers of $\delta\mathbf{M}_q$, we get a Feynman diagram expansion in terms of the renormalized propagators, as follows

$$\mathcal{F}_E = -\frac{1}{N_s\beta}\mathrm{Tr}\ln[-\underline{G}(k)^{-1}] - \left[\quad + \quad + \quad + \quad + \ldots\right] + \sum_q \frac{|M\hat{\mathbf{z}}\delta_q + \delta\mathbf{M}_q|^2}{2I}. \tag{13.222}$$

where the wavy line denotes scattering off the order-parameter fluctuations. Now since the action is stationary with respect to fluctuations, all terms linear in $\delta\mathbf{M}_q$ must cancel. which leads to

$$\Delta\mathcal{F}_E[\mathbf{M}] = -\left[\quad + \quad + \quad + \ldots\right] + \sum_q \frac{|\delta\mathbf{M}_q|^2}{2I}, \tag{13.223}$$

where $\Delta\mathcal{F}_E[\mathbf{M}] = \mathcal{F}_E[\mathbf{M}] - \mathcal{F}_E[\mathbf{M}^{(0)}]$. Only first diagram and the final term in this expression, are quadratic in $\delta\mathbf{M}_q$. Combining them, and dropping the higher order terms, we obtain the "Gaussian action" for the magnetization fluctuations

$$\begin{aligned}\Delta\mathcal{F}_G[\mathbf{M}] &= \frac{1}{2}\sum_q \delta M^a_{-q}\left[\frac{\delta_{ab}}{I} - \sigma^a \overset{k+q}{\underset{k}{\bigcirc}} \sigma^b\right]\delta M^b_q \\ &= \frac{1}{2}\delta M^a_{-q}\left[\frac{\delta_{ab}}{I} - \chi^{(0)}_{ab}(q)\right]\delta M^b_{-q}\end{aligned} \tag{13.224}$$

Gaussian Action of Fluctuations.

where

$$\chi^{(0)}_{ab}(q) = \sigma^a \overset{k+q}{\underset{k}{\bigcirc}} \sigma_b = -\frac{1}{\beta N_s}\sum_k \mathrm{Tr}\left[\sigma_a G(k+q)\sigma_b G(k)\right] \tag{13.225}$$

is the "bare" susceptibility of the polarized metal. Now the presence of a magnetization means that the off-diagonal terms $\chi^{(0)}_{xy}(q) = \chi^{(0)}_{yx}(-q)$ are non-zero. To diagonalize the magnetic fluctuations, it is convenient to work in terms of the raising and lowering components of the transverse spin, $\sigma_\pm = \frac{1}{2}(\sigma_x \pm i\sigma_y)$, and the corresponding components of the magnetization

$$M^\pm_q = M^x_q \pm iM^y_q.$$

The non-zero components of the transverse susceptibility are then

$$\begin{aligned}\chi^{(0)}_{+-}(q) &= -\frac{1}{\beta N_s}\sum_k \mathrm{Tr}\Big[\sigma_+ G(k+q)\sigma_- G(k)\Big]\\ \chi^{(0)}_{-+}(q) &= -\frac{1}{\beta N_s}\sum_k \mathrm{Tr}\Big[\sigma_- G(k+q)\sigma_+ G(k)\Big] = \chi^{(0)}_{+-}(-q)\end{aligned} \tag{13.226}$$

where the identity $\chi^{(0)}_{-+}(q) = \chi^{(0)}_{+-}(-q)$ follows by changing variables $k \to k-q$ inside the sum.

Rewriting $\mathbf{M}\cdot\boldsymbol{\sigma} = M^z_q\sigma_z + M^+\sigma_- + M^-\sigma_+$, the Gaussian effective action then becomes

$$\begin{aligned}\Delta\mathcal{F}_G[\mathbf{M}] &= \frac{1}{2}\sum_q\Big[\delta M^z_{-q}\Big(\frac{1}{I} - \chi^{(0)}_{zz}(q)\Big)\delta M^z_q\\ &+ \delta M^-_{-q}\Big(\frac{1}{2I} - \chi^{(0)}_{+-}(q)\Big)\delta M^+_q + \delta M^+_{-q}\Big(\frac{1}{2I} - \chi^{(0)}_{-+}(q)\Big)\delta M^-_q\Big]\end{aligned} \tag{13.227}$$

Now since the magnetization is a real variable, follows that $\overline{\delta M^\pm}_q = \delta M^\mp{}_{-q}$ (where we use a bar to denote complex conjugate) so we can rewrite this expression in the form

$$\begin{aligned}\Delta\mathcal{F}_G[\mathbf{M}] &= \frac{1}{2}\sum_q\Big[\delta M^z_{-q}\Big(\frac{1}{I} - \chi^{(0)}_{zz}(q)\Big)\delta M^z_q\\ &+ \overline{\delta M^+}_q\Big(\frac{1}{2I} - \chi^{(0)}_{+-}(q)\Big)\delta M^+_q + \delta M^+_{-q}\Big(\frac{1}{2I} - \chi^{(0)}_{-+}(q)\Big)\overline{\delta M^+}_{-q}\Big]\end{aligned} \tag{13.228}$$

It is this quadratic functional that provides the argument for the Gaussian distribution function of the magnetic fluctuations $p[M_q] = Z^{-1}e^{-\Delta S[\mathbf{M}]} = e^{-\beta N_s\Delta\mathcal{F}_G[\mathbf{M}]}$. Now by (13.226), $\chi^{(0)}_{-+}(q) = \chi^{(0)}_{+-}(q)$ so we can combine the last terms into one. The final results describing the distribution function for the Gaussian magnetic fluctuations about the Stoner mean-field theory for an intinerant ferromagnet are

$$p[M_q] \propto e^{-\Delta S[\mathbf{M}]} = e^{-\beta N_s\Delta\mathcal{F}_G[\mathbf{M}]} \tag{13.229}$$

$$\Delta\mathcal{F}_G[\mathbf{M}] = \sum_q\Big[\frac{1}{2}\delta M^z_{-q}\Big(\frac{1}{I} - \chi^{(0)}_{zz}(q)\Big)\delta M^z_q + \overline{\delta M^+}_q\Big(\frac{1}{2I} - \chi^{(0)}_{+-}(q)\Big)\delta M^+_q\Big]. \tag{13.230}$$

From the Gaussian form of this distribution, we can immediately read off the fluctuations in magnetization. Denoting

$$\langle\delta M^\alpha_q\delta M^\beta_{-q'}\rangle = \frac{1}{\beta N_s}\delta_{q,q'}\times\langle\delta M^\alpha_q\delta M^\beta_{-q}\rangle \tag{13.231}$$

the fluctuations in magnetization are given by

$$\begin{aligned}\langle\delta M^z_q\delta M^z_{-q}\rangle &= \frac{1}{\frac{1}{I} - \chi^{(0)}_{zz}(q)}\\ \langle\delta M^+_q\overline{\delta M^+}_{-q}\rangle &= \frac{1}{\frac{1}{2I} - \chi^{(0)}_{+-}(q)}\end{aligned} \tag{13.232}$$

Let us now convert these results into spin correlation functions. If we go back to the original Hubbard Stratonovich transformation, (13.182), we recall that to decouple the interaction, we had to introduce a dummy white noise variable, let us call it $\mathbf{m}_j(\tau)$, with distribution function $\langle m^a_j(\tau)m^b_j(\tau')\rangle = I\delta^{ab}\delta(\tau-\tau')$, or $\langle m^a_q m^b_{-q}\rangle = I\delta^{ab}$. To carry out the Hubbard Stratonovich transformation we redefined this varible, writing $\mathbf{m}_j(\tau) \to \mathbf{M}_j - I\boldsymbol{\sigma}_j$. It follows that the variable we are working with is related to the original white noise variable by $\mathbf{M}_j(\tau) = \mathbf{m}_j(\tau) + I\boldsymbol{\sigma}_j(\tau)$. Consequently, the Gaussian fluctuations in the magnetization are given by

$$\langle\sigma^a_q\sigma^b_{-q}\rangle = \frac{1}{I^2}\Big[\langle\delta M^a_q\delta M^b_{-q}\rangle - \overbrace{\langle\delta m^a_q\delta m^b_{-q}\rangle}^{I\delta^{ab}}\Big]$$

It follows that

$$\begin{aligned}\langle\sigma^z_q\sigma^z_{-q}\rangle &= \chi_{zz}(q) = \frac{1}{I^2}\Big[\frac{1}{\frac{1}{I} - \chi^{(0)}_{zz}(q)} - I\Big] = \frac{\chi^{(0)}_{zz}(q)}{1 - I\chi^{(0)}_{zz}(q)} \quad \text{(Longitudinal)}\\ \langle\sigma^+_q\sigma^-_{-q}\rangle &= \chi_{+-}(q) = \frac{1}{I^2}\Big[\frac{1}{\frac{1}{2I} - \chi^{(0)}_{+-}(q)} - 2I\Big] = \frac{\chi^{(0)}_{+-}(q)}{1 - 2I\chi^{(0)}_{+-}(q)} \quad \text{(Transverse)}\end{aligned} \tag{13.233}$$

RPA spin fluctuations

These are the celebrated "RPA" spin fluctuations of an intinerant Ferromagnet.

It is particularly interesting to examine the transverse spin fluctuations in (13.233). A uniform transverse spin fluctuation corresponds to a rotation of the magnetization, which costs no energy due to the rotational invariance of the system. If we carry out a slow twist of the magnetization, this costs an energy that goes to zero as the pitch of the twist goes to infinity. The corresponding normal mode is the "Goldstone mode" of the magnet.

One can analtyically calculate the transverse spin fluctuations of a ferromagnet with a quadratic dispersion $\epsilon_{\mathbf{k}} = \frac{k^2}{2m} - \mu$, because the bare susceptibilities $\chi^{(0)}(q)$ can be calculated as Lindhardt

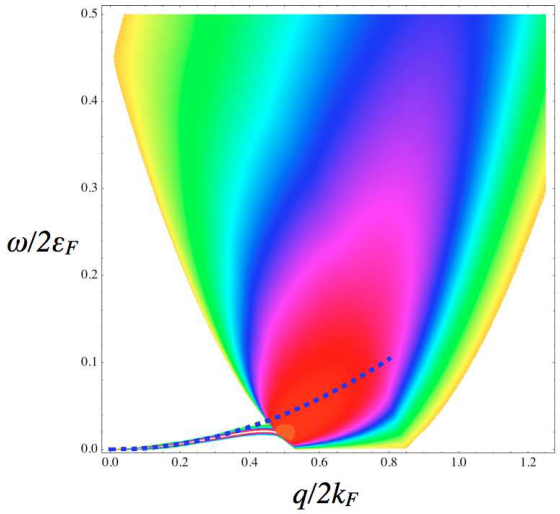
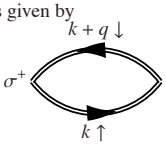


Figure 13.8: The energy spectrum of quantum magnetic fluctuations in an intinerant ferromagnet. The above spectrum was computed for a magnetization $M = 0.9\epsilon_F$ corresponding to an almost fully polarized Fermi sea.

functions. The transverse bare susceptibility (per unit cell) is given by

$$\begin{aligned}\chi^{(0)}_{+-}(q) &= -\frac{1}{N_s\beta}\sum_{\mathbf{k},i\omega_n}[\sigma_+ G(k+q)\sigma_- G(k)] = \sigma^+ \quad \sigma^- \\ &= -\frac{1}{N_s\beta}\sum_{\mathbf{k},i\omega_n}\Big[G_\downarrow(k+q)G_\uparrow(k)\Big] \\ &= a^3\int_{\mathbf{k}}\frac{f_{\mathbf{k}\uparrow}-f_{\mathbf{k}+\mathbf{q}\downarrow}}{(\epsilon_{\mathbf{k}+\mathbf{q}\downarrow}-\epsilon_{\mathbf{k}\uparrow})-i\nu_n}\end{aligned} \qquad (13.234)$$



where $\epsilon_{\mathbf{k}\sigma} = \epsilon_{\mathbf{k}} - \sigma M$, ($\sigma = \uparrow, \downarrow$). These sort of expressions are a type of Lindhard function already encountered in chapter 8. Following the same lines as section 8.62, we analytically continuing to real frequencies, and rewrite the integrals as follows

$$\chi^{(0)}_{+-}(\mathbf{q},\nu) = a^3\int_{\mathbf{k}}\left(\frac{f_{\mathbf{k}\uparrow}}{(\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}})-(\nu-2M)}+\frac{f_{\mathbf{k}\downarrow}}{(\epsilon_{\mathbf{k}-\mathbf{q}}-\epsilon_{\mathbf{k}})+(\nu-2M)}\right)$$

$$\begin{aligned}&= \sum_{\sigma=\pm}a^3\int_0^{k_{F\sigma}}\frac{k^2dk}{2\pi^2}\int\frac{d\cos\theta}{2}\left[\frac{1}{(\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}})-\sigma(\nu-2M)}\right] \\ &= \frac{1}{2}\sum_\sigma\left(\frac{mk_{F\sigma}}{\pi^2}\right)\mathcal{F}\left(\frac{q}{2k_{F\sigma}},\sigma\frac{\nu-2M}{4\epsilon_F}\right)\end{aligned} \qquad (13.235)$$

where $\epsilon_{F\sigma} = \epsilon_F + \sigma M$ and $k_{F\sigma} = k_F(1+\frac{M}{\epsilon_F})^{\frac{1}{2}}$ are the Fermi energy and momenta of the spin $\sigma = (\uparrow, \downarrow)$ Fermi surfaces and

$$\begin{aligned}\mathcal{F}[\tilde{q},\tilde{\nu}] &= \frac{1}{8\tilde{q}}\left[(1-A^2)\ln\left(\frac{A+1}{A-1}\right)+2A\right], \\ A &= \tilde{q}-\frac{\tilde{\nu}}{\tilde{q}}\end{aligned} \qquad (13.236)$$

is the Lindhard function.

Fig. (13.8) shows a density plot of the transverse dynamical spin susceptibility $\chi''_{+-}(\mathbf{q},\nu) = \mathrm{Im}\chi_{+-}(\mathbf{q},\nu-i\delta)$ predicted by the Gaussian (RPA) theory. The spectrum of magnetic fluctuations about the mean-field theory is determined by the energies at which one can excite a particle-hole pair by flipping a spin. Unlike a non-magnetic metal, the energy to flip a spin at $\mathbf{q} = 0$ is twice the Weiss field $\epsilon_{\mathbf{k}\downarrow} - \epsilon_{\mathbf{k}\uparrow} = 2M$. The continuum of spin-flip particle-hole excitations is thus lifted up at low momenta, forming what is known as the "Stoner continuum". The threshold energy for a spin-flip excitation finally drops to zero at the wavevector $q = k_{F\uparrow} - k_{F\downarrow}$. Below the Stoner continuum is a sharp Goldstone mode, labelled by the dotted line in Fig ()13.8), corresponding to a low-energy pole in the dynamic susceptibility located at frequencies $\omega_{\mathbf{q}}$ determined by the condition

$$2I\chi_{+-}(\mathbf{q},\omega_{\mathbf{q}}) = 1.$$

A careful evaluation of this condition shows that

$$\omega_{\mathbf{q}} = Z(M/\epsilon_F)\frac{q^2}{2m}, \qquad (13.237)$$

where

$$Z(x) = \frac{4}{5x}\left[\frac{(1+x)^{5/2}-(1-x)^{5/2}-5}{(1+x)^{3/2}-(1-x)^{3/2}}.\right] \qquad (13.238)$$

This is the relation used to determine the dotted line-curve in Fig. (13.8).

13.7 Summary

Casting many body quantum mechanics as a path integral. Key result. So second nature, that most condensed matter physicists use the same notation for the operators and their c-number representation inside the path integral.

With these approaches, one has to have the Hamiltonian in the form of canonical operators. Poses problems in strongly correlated systems, where the strong interactions between the particles

force us to introduce new operators that do not obey canonical commutation relations. We will return to these issues in Chapter ***.

As an example, we examined how these methods can be applied to itinerant ferromagnetism. In the process, we encountered the new concept of a "quantum phase transition", a point in the phase diagram where the long range order is destroyed by quantum, rather than thermal fluctuations. This is a subject of immense current interest Though we didn't follow it in detail, we remarked that the saddle point could be made exact in the large N limit of $1/N$ expansion. These methods are believed to break down in two dimensions (ref to Metilsky and Sun Silk Lee), and the resolution of this situation is at this time, an unsolved problem of great interest.

13.8 Appendices

Appendix 13A Derivation of key properties of bosonic coherent states.

Here we derive the matrix elements and the completeness properties of bosonic coherent states.

Matrix elements. Matrix elements of normal ordered operators $O[\hat{\mathfrak{b}}^\dagger, \hat{\mathfrak{b}}]$ between two coherent states are obtained simply by replacing the operators $\hat{\mathfrak{b}}$ and $\hat{\mathfrak{b}}^\dagger$ by the c-numbers b and $\bar{b}$ respectively:

$$\langle \bar{b}_1|\hat{O}[\hat{\mathfrak{b}}^\dagger, \hat{\mathfrak{b}}]|b_2\rangle = O[\bar{b}_1, b_2] \times \langle \bar{b}_1|b_2\rangle = O[\bar{b}_1, b_2] \times e^{\bar{b}_1 b_2} \tag{13.239}$$

To derive the matrix elements of coherent states, we first note that the properties of coherent states guarantee that

$$\langle \bar{b}|(\hat{\mathfrak{b}}^\dagger)^n \hat{\mathfrak{b}}^m|b\rangle = (\bar{b}^\dagger)^n b^m \langle \bar{b}|b\rangle = (\bar{b})^n b^m e^{\bar{b}b}. \tag{13.240}$$

Thus if $\hat{O}[\hat{\mathfrak{b}}^\dagger, \hat{\mathfrak{b}}] = \sum_{m,n} O_{mn} (\hat{\mathfrak{b}}^\dagger)^m b^n$ is a *normal ordered* operator, (all annihilation operators on the right), it follows that

$$\langle \bar{b}|\hat{O}[\hat{\mathfrak{b}}^\dagger, \hat{\mathfrak{b}}]|b\rangle = \sum_{m,n} O_{mn}\, \bar{b}^m b^n \times \langle \bar{b}|b\rangle = O[\bar{b}, b] \times e^{\bar{b}b}.$$

or

$$\hat{O}[b^\dagger, b] \xrightarrow{\text{coherent states}} O[\bar{b}, b] \times \langle \bar{b}|b\rangle$$

Note that if one has an operator that is not normal ordered, then one has to normal-order the operator prior to applying this theorem. For example, if $O = (\hat{\mathfrak{b}} + \hat{\mathfrak{b}}^\dagger)^2$, then $O =: O : +1$, and $\langle \bar{b}|O|b\rangle = [(b + \bar{b})^2 + 1]e^{\bar{b}b}$.

Completeness.

The unit operator can be decomposed in terms of coherent states as follows

$$\hat{1} = \sum_{\bar{b},b} |b\rangle\langle \bar{b}|, \tag{13.241}$$

where

$$\sum_{\bar{b},b} \equiv \int \frac{d\bar{b}db}{2\pi i} e^{-\bar{b}b} \tag{13.242}$$

is the normalized measure for summing over coherent states. To demonstrate the completeness relation, we will first derive the orthogonality relation between the wavefunctions $\phi_n(b) = \langle n|b\rangle$ of the coherent states:

$$I_{nm} = \int \frac{d\bar{b}db}{2\pi i} e^{-\bar{b}b} \langle n|b\rangle\langle \bar{b}|m\rangle = \delta_{nm}. \tag{13.243}$$

To prove this, let us substitute $b = re^{i\phi}$ and $\bar{b} = re^{-i\phi}$. Although $\bar{b}$ and b are complex conjugates of each other, they are derived from two independent real variables, and so the measure for integrating over them is two-dimensional. We can transform the measure into polar co-ordinates by introducing a Jacobian, as follows:

$$d\bar{b}db = \overbrace{\left\| \begin{matrix} \frac{\delta\bar{b}}{\delta r} & \frac{\delta\bar{b}}{\delta\phi} \\ \frac{\delta b}{\delta r} & \frac{\delta b}{\delta\phi} \end{matrix} \right\|}^{\delta[\bar{b},b]/\delta[r,\phi]} drd\phi = \left\| \begin{matrix} e^{-i\phi} & -ire^{-i\phi} \\ e^{i\phi} & ire^{i\phi} \end{matrix} \right\| drd\phi = 2irdrd\phi$$

so that (13.243) factorizes into a radial and an angular integral,

$$I_{nm} = \frac{1}{\sqrt{n!m!}} \int \frac{d\bar{b}db}{2\pi i} \bar{b}^n \bar{b}^m e^{-\bar{b}b} = \frac{1}{\sqrt{n!m!}} \int_0^\infty 2rdr r^{n+m} e^{-r^2} \times \overbrace{\int_0^{2\pi} \frac{d\phi}{2\pi} e^{i\phi(n-m)}}^{\delta mn} \tag{13.244}$$

where we have substituted $\langle n|b\rangle = \frac{1}{\sqrt{n!}} b^n$ and $\langle \bar{b}|m\rangle = \frac{1}{\sqrt{m!}} \bar{b}^m$. The angular integral vanishes unless $n = m$. Changing variables $r^2 \to x$, $2rdr = dx$ in the first integral we then obtain

$$I_{nm} = \frac{\delta_{nm}}{n!} \int_0^\infty dx\, x^n e^{-x} = \delta_{nm} \tag{13.245}$$

proving the orthogonality relation. Now since $\delta_{nm} = \langle n|m\rangle$, we can write the orthogonality relation (13.243) as

$$\langle n|m\rangle = \int \frac{d\bar{b}db}{2\pi i} e^{-\bar{b}b} \langle n|b\rangle\langle \bar{b}|m\rangle = \langle n| \left(\int \frac{d\bar{b}db}{2\pi i} e^{-\bar{b}b} |b\rangle\langle \bar{b}| \right) |m\rangle.$$

Since this holds for all states $|n\rangle$ and $|m\rangle$, it follows that the quantity in brackets is the unit operator,

$$\hat{1} = \int \frac{d\bar{b}db}{2\pi i} e^{-\bar{b}b} |b\rangle\langle \bar{b}| = \int \frac{d\bar{b}db}{2\pi i} \frac{|b\rangle\langle \bar{b}|}{\langle \bar{b}|b\rangle} \equiv \sum_{\bar{b},b} |b\rangle\langle \bar{b}| \tag{13.246}$$

Completeness relation

Appendix 13B Grassman Differentiation and Integration

Differentiation is defined to have the normal linear properties of the differential operator. We denote

$$\partial_c \equiv \frac{\partial}{\partial c}, \quad \partial_{\bar{c}} \equiv \frac{\partial}{\partial \bar{c}} \tag{13.247}$$

so that

$$\partial_c c = \partial_{\bar{c}} \bar{c} = 1. \tag{13.248}$$

If we have a function

$$f(\bar{c}, c) = f_0 + \bar{f}_1 c + \bar{c} f_1 + f_{12} \bar{c} c \tag{13.249}$$

then differentiation from the left-hand side gives

$$\begin{aligned} \partial_c f &= \bar{f}_1 - f_{12} \bar{c} \\ \partial_{\bar{c}} f &= f_1 + f_{12} c \end{aligned} \tag{13.250}$$

where the minus sign in the first expression occurs because the $\bar{\partial}$ operator must anticommute with c. But how do we define integration? This proves to be much easier for Grassman variables, than for regular c-numbers. The great sparseness of the space of functions dramatically restricts the number of linear operations we can apply to functions, forcing differentiation and integration to become the *same* operation :

$$\int dc \equiv \partial_c, \qquad \int d\bar{c} \equiv \partial_{\bar{c}} \tag{13.251}$$

In other words,

$$\int d\bar{c}\bar{c} = 1, \qquad \int dcc = 1, \qquad \int d\bar{c} = \int dc = 0 \tag{13.252}$$

Appendix 13C Grassman calculus: Change of variables

Suppose we change variables, writing

$$\begin{pmatrix} c_1 \\ \vdots \\ c_r \end{pmatrix} = A \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_r \end{pmatrix} \tag{13.253}$$

where A is c-number matrix, then we would like to know how to evaluate the Jacobian for this transformation, which is defined so that

$$\int dc_1 \ldots dc_r \, [\ldots] = \int J\left(\frac{c_1 \ldots c}{\xi_1 \ldots \xi_r}\right) d\xi_1 \ldots d\xi_r \, [\ldots] \tag{13.254}$$

Now since integration and differentiation are identical for Grassman variables, we can evaluate the fermionic Jacobian using the chain rule for differentiation, as follows

$$\begin{aligned} \int dc_1 \ldots dc_r \, [\ldots] &= \frac{\partial^r}{\partial c_1 \ldots \partial c_r} [\ldots] \\ &= \sum_P \left(\frac{\partial \xi_{P_1}}{\partial c_1} \ldots \frac{\partial \xi_{P_r}}{\partial c_r} \right) \frac{\partial^r}{\partial \xi_{P_1} \ldots \partial \xi_{P_r}} [\ldots] \end{aligned} \tag{13.255}$$

where $P = \begin{pmatrix} 1 & \ldots & r \\ P_1 & \ldots & P_r \end{pmatrix}$ is a permutation of the sequence $(1 \ldots r)$. But we can order the differentiation in the second term, picking up a factor $(-1)^P$ where P is the signature of the permutation, to obtain

$$\begin{aligned} \int dc_1 \ldots dc_r \, [\ldots] &= \sum_P (-1)^P \left(\frac{\partial \xi_{P_1}}{\partial c_1} \ldots \frac{\partial \xi_{P_r}}{\partial c_r} \right) \frac{\partial^r}{\partial \xi_1 \ldots \partial \xi_r} [\ldots] \\ &= \mathrm{Det}[A^{-1}] \frac{\partial^r}{\partial \xi_1 \ldots \partial \xi_r} [\ldots] \\ &= \int \mathrm{Det}[A^{-1}] d\xi_1 \ldots d\xi_r \, [\ldots] \end{aligned} \tag{13.256}$$

where we have recognized the prefactor as the determinant of the inverse transformation $\xi = \underline{A}^{-1} c$. From this result, we can read off the Jacobian of the transformation as

$$J\left(\frac{c_1 \ldots c_r}{\xi_1 \ldots \xi_r}\right) = \mathrm{Det}[A]^{-1} = \left| \frac{\partial c_1 \ldots c_r}{\partial \xi_1 \ldots \xi_r} \right|^{-1} \tag{13.257}$$

which is precisely the inverse of the bosonic Jacobian. This has important implications for supersymmetric field theories, where the Jacobian of the bosons and fermions precisely cancel. For our purposes however, the most important point, is that for a Unitary transformation, the Jacobian is unity.

Appendix 13D Grassman Calculus: Gaussian Integrals

The basic Gaussian integral is simply

$$\int d\bar{c}dce^{-a\bar{c}c} = \int d\bar{c}dc(1 - a\bar{c}c) = a \tag{13.258}$$

If now we introduce a set of N variables, then

$$\int \prod_j d\bar{c}_j dc_j \exp -[\sum_j a_j \bar{c}_j c_j] = \prod_j a_j \tag{13.259}$$

Suppose now, we carry out a unitary transformation, for which the Jacobian is unity, then since

$$c = U\xi, \qquad \bar{c} = \bar{\xi}U^\dagger,$$

the integral then becomes

$$\int \prod_j d\bar{\xi}_j d\xi_j \exp[-\bar{\xi} \cdot A \cdot \xi] = \prod_j a_j$$

where $A_{ij} = \sum_l U^\dagger{}_{il} a_l U_{lj}$ is the matrix with eigenvalues a_l. It follows that

$$\int \prod_j d\bar{\xi}_j d\xi_j \exp[-\bar{\xi} \cdot A \cdot \xi] = \mathrm{Det}[A] \tag{13.260}$$

Finally, by shifting the variables $\xi \to \xi + A^{-1} j$, where j is an arbitrary vector, we find that

$$\boxed{Z[j] = \int \prod_j d\bar{\xi}_j d\xi_j \exp[-(\bar{\xi} \cdot A \cdot \xi + \bar{j} \cdot \xi + \bar{\xi} \cdot j)] = \mathrm{Det}[A] \exp[\bar{j} \cdot A^{-1} \cdot j]} \tag{13.261}$$

This is the basic Gaussian integral for Grassman variables. Notice that using the result $\ln\mathrm{Det}[A] = \mathrm{Trln}[A]$, it is possible to take the logarithm of both sides to obtain

$$S[j] = -\ln Z[j] = -\mathrm{Trln}[A] - \bar{j} \cdot A^{-1} \cdot j. \tag{13.262}$$

The main use of this integral, is for evaluating the Path integral for free field theories. In this case, the matrix $A \to -G^{-1}$ becomes the inverse propagator for the fermions, and $\xi_n \to \psi(i\omega_n)$ is the Fourier component of the Fermi field at Matsubara frequency $i\omega_n$.

13.9 Exercises

1. In this problem consider $\hbar = 1$. Suppose $|0\rangle$ is the ground-state of a harmonic oscillator problem, where $b|0\rangle = 0$. Consider the state formed by simultaneously translating this state in momentum and position space as follows:
$$|p, x\rangle = \exp\left[-i(x\hat{p} - p\hat{x})\right]|0\rangle.$$
By rewriting $\hat{b} = (\hat{x} + i\hat{p})/\sqrt{2}, z = (x + ip)/\sqrt{2}$, show that this state can be rewritting as
$$|p, x\rangle = e^{b^\dagger z - \bar{z}b}|0\rangle$$
Using the relation $e^{A+B} = e^A e^B e^{\frac{1}{2}[A,B]}$, provided $[A, [A, B]] = [B, [A, B]] = 0$, show that $|p, x\rangle$ is equal to a normalized coherent state
$$|p, x\rangle \equiv |z\rangle e^{-\bar{z}z/2} = e^{b^\dagger z}|0\rangle e^{-\frac{1}{2}\bar{z}z}$$
showing that the coherent state $|z\rangle$ represents a minimum uncertainty wavepacket centered at (q, p) in phase space.

2. Repeat the calculation of section 13.33. without taking the continuum limit. Show that the path integral for a single boson with Hamiltonian $H = \epsilon b^\dagger b$ with a large, but finite number of time slices is given by
$$\ln Z_N = \sum_{n=1}^{N} \ln\Big(\epsilon - i\nu_n F(\nu_n \Delta\tau/2)\Big)$$
where $F(x) = (1 - e^{-x})/x$. If you approaximate each term in the sum by its value at $\Delta\tau = 0$, and then take $N \to \infty$ the result obviously converges to the continuum limit. But the error contribution from N such terms appears to be of order $O(N \times \Delta\tau) = O(1)$. Use contour integration to show that this is fortunately an over-estimate, and that the actual error is $O(\Delta\tau) = O(1/N)$.

3. Using path integrals, calculate the partition function for a single Zeeman-split electronic level described by the action
$$S = \int d\tau \bar{f}_\alpha \Big(\delta_{\alpha\beta}\partial_\tau + \boldsymbol{\sigma}_{\alpha\beta} \cdot \boldsymbol{B}\Big) f_\beta$$
Why is your answer not the same as the partition function of a spin $S = 1/2$ in a magnetic field?

4. Suppose
$$\mathcal{M} = e^{\frac{1}{2}\sum_{i,j} A_{ij} c^\dagger{}_i c^\dagger{}_j}$$
where A_{ij} is an $N \times N$ antisymmetric matrix, and the $c^\dagger{}_j$ are a set of N canonical Fermi creation operators. Using coherent states, calculate
$$\mathrm{Tr}[\mathcal{M}\mathcal{M}^\dagger]$$
where the trace is over the 2^N dimensional Hilbert space of fermions. (Hint: notice that $\mathcal{M}\mathcal{M}^\dagger$ is already normal ordered, so that by using the trace formula, you can rewrite this in terms of a simple Grassman integral.)

5. Calculate, to Gaussian order, the change in the BCS effective action for a fluctuation in the gap function of the following form
$$\Delta(\tau) = \Delta_0 + \frac{1}{\sqrt{\beta}} \sum_n \delta\Delta_n e^{-i\nu_n \tau}$$

where $\nu_n = 2\pi T n$ is the Bose Matsubara frequency and Δ_0 is a value of Δ which minimizes the effective action. Use your result to confirm that the BCS Free energy per unit volume is accurate to $O(1/V)$, where V is the volume.

6. Re-derive table 1. for the case of bosonic coherent states.

$$|b\rangle = e^{bb^\dagger}|0\rangle$$

where the Grassman variable is now replaced by a conventional c-number b.

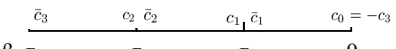
7. (a) Suppose $H = \epsilon c^\dagger c$ represents a single fermion state. Consider the approximation to the partition function obtained by dividing up the period $\tau \in [0, \beta]$ into N equal time-slices,

$$Z_N = \mathrm{Tr}[(e^{-\Delta\tau H})^N] \tag{13.263}$$

where $\Delta\tau = \beta/N$. By using coherent states $|c\rangle = e^{\hat{c}^\dagger c}|0\rangle$, and approximating the matrix element from time τ_j to time τ_{j+1}, where $\tau_j = j\Delta\tau$ by

$$\langle \bar{c}_{j+1}|e^{-\Delta\tau H}|c_j\rangle = e^{\alpha\bar{c}_{j+1}c_j} + O(\Delta\tau^2) \tag{13.264}$$

where $\alpha = (1 - \Delta\tau\epsilon)$, (Fig. 1.)



(13.265)

show that Z_3 can be written as a "toy functional integral",

$$Z_3 = \int d\bar{c}_3 dc_3 d\bar{c}_2 dc_2 d\bar{c}_1 dc_1 \exp\left\{-(\bar{c}_3, \bar{c}_2, \bar{c}_1)\begin{bmatrix}1 & -\alpha & 0\\ 0 & 1 & -\alpha\\ \alpha & 0 & 1\end{bmatrix}\begin{pmatrix}c_3\\ c_2\\ c_1\end{pmatrix}\right\} \tag{13.266}$$

(b) Evaluate Z_3.

(c) Generalize the result to N time slices and obtain an expression for Z_N. What is the limiting value of your result as $N \to \infty$?

8. Derive the completeness and trace formulae for a set of bosonic coherent states,

$$|\alpha\rangle = e^{b^\dagger \alpha}|0\rangle \tag{13.267}$$

You may assume the basic result

$$\delta_{nm} = \int \frac{d\bar{b}db}{2\pi i} e^{-\bar{b}b} b^n \bar{b}^m$$

In particular

(a) Show that the completeness relation is given by

$$\sum_{|b\rangle,\,|\bar{b}\rangle} |b\rangle\langle\bar{b}| = 1$$
$$\sum_{|b\rangle,\,|\bar{b}\rangle} = \int \frac{d\bar{b}db}{2\pi i} e^{-\bar{b}b} \tag{13.268}$$

(b) Show that the trace formula is given by

$$Tr[\hat{A}] = \sum_{|b\rangle,\,|\bar{b}\rangle} \langle\bar{b}|\hat{A}|b\rangle$$

(c) What is the key difference between the derivation of the Bosonic and the Fermionic path integrals?

9. The one dimensional electron gas is prone to the development of charge-density wave instabilities. The treatment of these instabilities bears close resemblance to the BCS theory of superconductivity. Suppose we have a one-dimensional conductor, described by the Hamiltonian

$$\begin{aligned} H - \mu N &= H_o + H_I, \\ H_o &= -t\sum_{j,\,\sigma}\left(\psi^\dagger{}_{j+1\,\sigma}\psi_{j\,\sigma} + \psi^\dagger{}_{j\,\sigma}\psi_{j+1\,\sigma}\right), \\ H_I &= -g\sum_j n_{j\uparrow}n_{j\downarrow} \end{aligned} \tag{13.269}$$

where $g > 0$ and $\psi^\dagger{}_{j\sigma}$ creates an electron with spin $\sigma = \pm\frac{1}{2}$ at site j. The separation between sites is taken to be unity and the chemical potential has been chosen to be zero, giving a half-filled band.

(a) Show that H_o can be diagonalized in the form

$$H_o = -\sum_{k\,\sigma}(2t\cos k)c^\dagger{}_{k\sigma}c_{k\sigma}, \tag{13.270}$$

where $c_{k\sigma} = \frac{1}{\sqrt{N}}\sum_j \psi_{j\sigma}e^{-ikj}$, $k = \frac{2\pi}{N}(0,\ 1,\ \ldots N-1)$. Please note that the band is exactly half-filled, so that the Fermi surfaces are separated by a distance π in momentum space and the average electron density is 1 per site.

(b) Suppose a staggered potential $V_j = -(-1)^j\Phi$ is applied to the conductor. This will induce a staggered charge density to the sample

$$\langle n_{j\sigma}\rangle = \frac{1}{2} + (-1)^j\Delta_j/g \tag{13.271}$$

At low temperatures, the staggered order will remain even after the applied potential is removed. Why? If the RMS fluctuations in the staggered charge density can be ignored, show that the interaction Hamiltonian can be recast in the form

$$H_I \to \sum_j\left((-1)^j\Delta_j\hat{n}_j + \frac{\Delta_j^2}{g}\right) + O(\delta\hat{n}_j^2). \tag{13.272}$$

(c) How can the above transformation be elevated to the status of an exact result using a path integral? (Note that the order parameter is no longer complex- does this change your discussion?)

(d) Calculate the excitation spectrum in the presence of the uniformly staggered order parameter $\Delta_j = \Delta$. (Hint: write the mean field Hamiltonian in momentum space and treat the terms that scatter from one-side of the Fermi surface in an analogous fashion to the pairing terms in superconductivity. You may find it useful to work with the spinor $\Psi_{k\sigma} = \begin{pmatrix} c_{k\sigma} \\ c_{k+\pi\sigma}\end{pmatrix}$.)

(e) Calculate the Free energy $F[\Delta]$ and sketch your result as a function of temperature. Write down the gap equation for the value of $\Delta(T)$ that develops spontaneously at low temperatures.

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Chapter 14

Superconductivity and BCS theory

14.1 Introduction: Superconductivity pre-history

As a specific illustration of the above approach, we shall now develop the BCS theory of superconductivity using the path integral method.

Before we start, a brief diversion about the history of superconductivity. Superconductivity - the phenomenon whereby the resistance of metal spontaneously drops to zero upon cooling below its critical temperature, was discovered by Kamerlingh Onnes in 1906. However, it took more than 50 years to fully develop the conceptual framework required to understand this collective phenomenon. During this time, many great physicists, including Bohr, Pauli and Feynman tried, yet failed to develop a microscopic theory of the phenomenon.

Some highlights in the development of the theory of superconductivity were

- Discovery of the Meissner effect in 1933 by Meissner and Ochsenfeld. When a superconductor is cooled in a small magnetic field, the flux is spontaneously excluded as it becomes superconducting. The Meissner effect demonstrates that a superconductor is, in essence a perfect diamagnet.

- London's observation in 1937, that perfect diamagnetism develops if the wavefunction develops a rigidity which prevents the paramagnetic component of the current evolving to screen out the diamagnetic current. (See earlier discussions) Using this reasoning, London deduced the famous relationship

$$\vec{j} = -\frac{n_s e^2}{m}\vec{A}, \qquad (\vec{\nabla}\cdot A = 0).$$

- Development of the Landau Ginzburg theory in 1951. Landau and Ginzburg extended the Landau theory of phase transitions, proposing that superconductivity involves a complex order parameter $\Psi(x)$. Using arguments of gauge invariance, LG reasoned that the Free energy must contain a gradient term of the form

$$f = \int d^3x \frac{1}{2m^*}|(-i\hbar\vec{\nabla} - e^*\vec{A})\psi(x)|^2$$

Although we now know that $e^* = 2e$, in the original version of the theory, Landau erroneously convinced Ginzburg that he had an argument based on gauge invariance, that proves $e^* = e$. The vitally important aspect of this free energy function is that once $\psi \neq 0$, the electromagnetic field develops a mass giving rise to a super-current

$$\vec{j} = -\frac{\delta f}{\delta \vec{A}(x)} = -\frac{(e^*)^2}{m^*}|\psi|^2\vec{A}(x)$$

The BCS Hamiltonian is one of the earliest examples of "model Hamiltonians". By the early fifties, the observation of the isotope effect by Bernie Serin at Rutgers University, had lead to the realization that the mechanism of superconductivity in conventional metals was driven by the electron phonon interaction. Frohlich had proposed his Hamiltonian for the electron phonon interaction, and had discovered that these interactions can give rise to sliding charge density waves. Frohlich's theoretical prediction of charge density waves was twenty five years ahead of its time, but it also misled him into thinking that charge density waves could provide the explanation of the Meissner effect. Frohlich's error was to neglect the effect of pining, which in any disordered materials, prevents incommensurate charge density waves from sliding freely.

In the early fifties, Bardeen and Pine's recognized that to make progress with the theory of superconductivity, it would be necessary to simplify the Hamiltonian by carrying out a canonical transformation that eliminates the phonon degrees of freedom, giving rise to an effective electron-electron interaction. The Bardeen Pine Hamiltonian is the immediate predecessor of the BCS model

14.2 The BCS Hamiltonian

We start with the BCS Hamiltonian

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \frac{g_0}{V} A^\dagger A$$

where

$$A = \sum_{\mathbf{k},|\epsilon_{\mathbf{k}}|<\omega_D} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}, \qquad A^\dagger = \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow},$$

are the operators that annihilate or create a uniform pair density. Note how the interaction between electrons is limited to within an energy ω_D of the Fermi energy. This "simplified" pairing Hamiltonian is the one originally used by BCS. Notice how the interaction

$$H_I = -\frac{g_0}{V}\sum_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow},$$

involves pairs of infinite spatial extent (all momenta summed over). This feature enhances the mean-field properties of the model to the point where mean-field theory actually gives the exact solution.

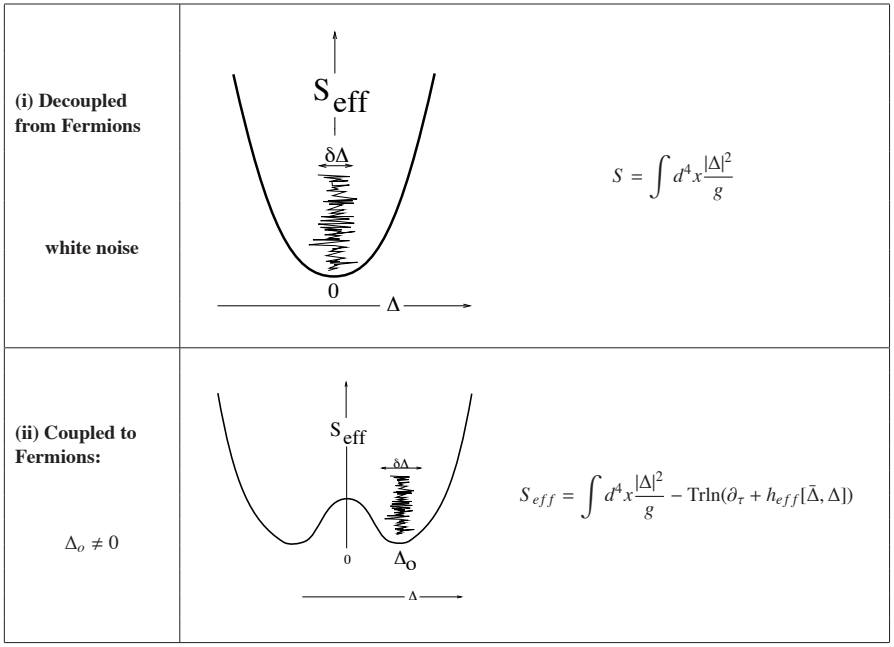


Fig. 3 Effective action for auxilliary field.

The volume normalizing factor $1/V$ is required so that this term grows linearly, rather than quadratically with volume V. We shall redefine $g = g_0/V$ to simplify our maniupations, re-instating the volume at the end of the calculation.

The appearance of just one A and $A^\dagger$ in the Hamiltonian makes it particularly easy to apply the methods introduced in the last section. We begin by writing the problem as a path integral

$$Z = \int \mathcal{D}[\bar{c}, c] e^{-S}$$

where

$$S = \int_0^\beta \sum_{\mathbf{k}\sigma} \bar{c}_{\mathbf{k}\sigma}(\partial_\tau + \epsilon_{\mathbf{k}}) c_{\mathbf{k}\sigma} - g\bar{A}A$$

Next we introduce the identity

$$\int \mathcal{D}[\bar{\Delta}, \Delta] \exp\Big[\frac{1}{g}\int_0^\beta d\tau \bar{\Delta}(\tau)\Delta(\tau)\Big] = 1 \tag{14.1}$$

into the path integral. By shifting the variables $\Delta \to \Delta + gA$, $\bar{\Delta} \to \bar{\Delta} + g\bar{A}$, we obtain

$$\begin{aligned} Z &= \int \mathcal{D}[\bar{\Delta}, \Delta, \bar{c}, c] e^{-S} \\ S &= \int_0^\beta d\tau \left\{ \sum_{\mathbf{k}\sigma} \bar{c}_{\mathbf{k}\sigma}(\partial_\tau + \epsilon_{\mathbf{k}}) c_{\mathbf{k}\sigma} + \Delta A + \bar{A}\Delta + \frac{1}{g}\bar{\Delta}\Delta \right\} \end{aligned} \tag{14.2}$$

where $\Delta(\tau)$ is a function of time only. In a Nambu notation, this can be re-written

$$S = \int_0^\beta d\tau \left\{ \sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}}(\partial_\tau + \underline{h}_{\mathbf{k}})\psi_{\mathbf{k}} + \frac{1}{g}\bar{\Delta}\Delta \right\} \tag{14.3}$$

where

$$\psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ \bar{c}_{-\mathbf{k}\downarrow} \end{pmatrix} \tag{14.4}$$

defines the Nambu spinor and

$$\underline{h}_{\mathbf{k}} = \begin{bmatrix} \epsilon_{\mathbf{k}} & \Delta(\tau) \\ \bar{\Delta}(\tau) & -\epsilon_{\mathbf{k}} \end{bmatrix} = \epsilon_{\mathbf{k}}\tau_3 + \Delta_1\tau_1 + \Delta_2\tau_2 \tag{14.5}$$

is the matrix Hamiltonian, where $\Delta = \Delta_1 - i\Delta_2$, $\bar{\Delta} = \Delta_1 + i\Delta_2$, and (τ_1, τ_2, τ_3) are the three Pauli matrices. (By convention the symbol τ is used to denote an "isospin" from a conventional spin.) Notice that the action is now quadratic in the Fermi fields, so we can formally carry out the Gaussian integral of the Fermi fields, "integrating out" the Fermions to obtain

$$e^{-S_{eff}[\bar{\Delta},\Delta]} = \prod_{\mathbf{k}} \det[\partial_\tau + \underline{h}_{\mathbf{k}}(\tau)] e^{-\int_0^\beta d\tau \frac{\bar{\Delta}\Delta}{g}}$$

for the effective action, where we have separated the fermionic determinant into a product over each decoupled momentum. Thus

$$S_{eff}[\bar{\Delta}, \Delta] = \int_0^\beta d\tau \frac{\bar{\Delta}\Delta}{g} + \sum_{\mathbf{k}} \mathrm{Trln}(\partial_\tau + \underline{h}_{\mathbf{k}}).$$

where we have replaced lndet $\to$ Trln. Except for certain uniform, or almost uniform configurations of Δ, we can not calculate S_{eff} explicitly. It turns out however, that these configurations dominate the path integral in the limit $V \to \infty$. To see this consider the path integral

$$Z = \int \mathcal{D}[\bar{\Delta}, \Delta] e^{-S_{eff}[\bar{\Delta},\Delta]}$$

The effective action is actually extensive in the volume, V, so that as $V \to \infty$, S/V is a constant. This means that when we find the configuration of $\Delta = \Delta_o$ which minimizes S_{eff}, the cost of fluctuations $\delta\Delta$ around this configuration will also be of order $O(V)$, i.e. the amplitude for a small fluctuation is given by

$$e^{-S} = e^{-S_o + O(V)\times|\delta\Delta|^2}$$

The appearance of V in the coefficient of this Gaussian distribution implies the variance of small fluctuations around the minimum will be of order O(1/V), so that to a good approximation,

$$Z = e^{-S_{eff}[\bar{\Delta}_o, \Delta_o] + O(1)}$$

This is why the mean-field approximation to the path integral is essentially exact for the BCS model.

Since the original problem is translationally invariant, we expect the configurations that minimize the action to also be uniform. The mean-field approximation to the path integral is made by replacing the integral over the Δ field by its uniform "saddle-point" value, obtained by replacing $\Delta(\tau)$ with a uniform field $\Delta(\tau) = \Delta_1 - i\Delta_2$. In this case, we can use momentum and frequency eigenstates for the Nambu fields

$$\psi_{\mathbf{k}}(\tau) = \frac{1}{\sqrt{\beta}} \sum_n \psi_{\mathbf{k}n} e^{-i\omega_n \tau}$$

In this basis,

$$\partial_\tau + h \to [-i\omega_n + \underline{h}_{\mathbf{k}}]$$

so that the determinant

$$\det[\partial_\tau + \underline{h}_{\mathbf{k}}] = \prod_n \det[-i\omega_n + \underline{h}_{\mathbf{k}}] = \prod_n [\omega_n^2 + \epsilon_{\mathbf{k}}^2 + |\Delta|^2]$$

and the effective action for a uniform field is

$$F_{eff} = \frac{S_{eff}}{\beta} = -T \sum_{\mathbf{k}n} \ln[\omega_n^2 + \epsilon_{\mathbf{k}}^2 + |\Delta|^2] + \frac{|\Delta|^2}{g}$$

We see that this is nothing more than the mean-field free-energy for the BCS model. Minimizing F_{eff} w.r.t Δ gives us the gap equations

$$\frac{\partial F_{eff}}{\partial \bar{\Delta}} = -\sum_{\mathbf{k}n} \frac{\Delta}{\omega_n^2 + E_{\mathbf{k}}^2} + V\frac{\Delta}{g_0} = 0 \tag{14.6}$$

or

$$\boxed{\frac{1}{g_0} = \frac{1}{\beta V} \sum_{\mathbf{k}n} \frac{1}{\omega_n^2 + E_{\mathbf{k}}^2} \qquad \text{BCS Gap equation}} \tag{14.7}$$

where

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta|^2}$$

is the quasiparticle energy and we have re-instated $g_0 = g/V$. This is the BCS gap equation.

Actually, for most of our purposes, it proves easier to manipulate the Free energy in its discrete, Matsubara form. We can in fact carry out the Matsubara sum at any stage in the above manipulation. Using the contour integration method,

$$F_{eff} = -\sum_{\mathbf{k}} \oint \frac{dz}{2\pi i} f(z) \ln[z^2 - E_{\mathbf{k}}^2] + V\frac{|\Delta|^2}{g_0}$$

where the integral runs anti-clockwise around the poles of the Fermi function. The logarithm inside the integral can be split up into two terms

$$\ln[z^2 - E_{\mathbf{k}}^2] \to \ln[E_{\mathbf{k}} - z] + \ln[-E_{\mathbf{k}} - z]$$

which we immediately recognize as the contributions from fermions with energies $\pm E_{\mathbf{k}}$, so that the result of carrying out the contour integral, is

$$\begin{aligned} F_{eff} &= -TV \int \frac{d^3k}{(2\pi)^3} \Big[\ln[1 + e^{-\beta E_{\mathbf{k}}}] + \ln[1 + e^{\beta E_{\mathbf{k}}}]\Big] + V\frac{|\Delta|^2}{g_0} \\ &= -2TV \int_{|\epsilon_{\mathbf{k}}|<\omega_D} \frac{d^3k}{(2\pi)^3} \Big[\ln[2\cosh(\beta E_{\mathbf{k}}/2)]\Big] + V\frac{|\Delta|^2}{g_0} \end{aligned} \tag{14.8}$$

Differentiating w.r.t. $\bar{\Delta}$ and setting $\partial F_{eff}/\partial\bar{\Delta} = 0$, then gives

$$\boxed{\frac{1}{g_0} = \int_{|\epsilon_{\mathbf{k}}|<\omega_D} \frac{d^3k}{(2\pi)^3} \Big[\frac{\tanh(\beta E_{\mathbf{k}}/2)}{2E_{\mathbf{k}}}\Big]} \tag{14.9}$$

If we approximate the density of states by a constant $N(0)$ per spin over the narrow shell of states around the Fermi surface, we may replace the momentum sum by an energy integral

$$\frac{1}{g_0} = N(0) \int_0^{\omega_D} d\epsilon \Big[\frac{\tanh(\beta\sqrt{\epsilon^2 + \Delta^2}/2)}{\sqrt{\epsilon^2 + \Delta^2}}\Big]. \tag{14.10}$$

14.3 Computing T_c

To compute T_c we shall take the Matsubara form of the gap equation (14.7), which we rewrite replacing the sum over momenta by an integral near the Fermi energy, replacing $\frac{1}{V}\sum_{\mathbf{k}} \to N(0)\int d\epsilon$ we get

$$\frac{1}{g_0} = TN(0) \sum_n \int_{-\infty}^{\infty} d\epsilon \frac{1}{\omega_n^2 + \epsilon_{\mathbf{k}}^2 + \Delta^2} = \pi TN(0) \sum_{|\omega_n|<\omega_D} \frac{1}{\sqrt{\omega_n^2 + \Delta^2}}$$

where we have extended the limits of integration over energy to infinity. By carrying out the integral over energy first, we are forced to impose the cut-off on the Matsubara frequencies.

If we now take $T \to 0$ in this expression, we may replace

$$T\sum_{\omega_n} = T\sum \frac{\Delta\omega_n}{2\pi T} \to \int \frac{d\omega}{2\pi} \tag{14.11}$$

so that at zero temperature and set $T = 0$, we obtain

$$1 = gN(0)\int_0^{\omega_D} \frac{d\epsilon}{\sqrt{\epsilon^2+\Delta^2}} = gN(0)\left[\sinh^{-1}\left(\frac{\omega_D}{\Delta}\right)\right] \approx gN(0)\ln\left(\frac{2\omega_D}{\Delta}\right)$$

where we have assumed $gN(0)$ is small, so that $\omega_D/\Delta >> 1$. We may now solve for the zero temperature gap, to obtain

$$\boxed{\Delta = 2\omega_D e^{-\frac{1}{gN(0)}}} \tag{14.12}$$

To calculate the transition temperature, we note that just below the transition temperature, the gap becomes infinitesimally small, so that $\Delta(T_c^-) = 0$. Substituting this into (14.11), we obtain

$$\frac{1}{gN(0)} = \pi T_c \sum_{|\omega_n|<\omega_D} \frac{1}{|\omega_n|} = 2\pi T_c \sum_{n=0}^{\infty}\left(\frac{1}{\omega_n} - \frac{1}{\omega_n+\omega_D}\right)$$

where we have imposed the limit on ω_n by subtracting off an identical term, with $\omega_n \to \omega_n + \omega_D$. Simplifying this expression gives

$$\frac{1}{gN(0)} = \sum_{n=0}^{\infty}\left(\frac{1}{n+\frac{1}{2}} - \frac{1}{\omega_n+\frac{1}{2}+\frac{\omega_D}{2\pi T_c}}\right)$$

At this point we can use an extremely useful identity of the digamma function $\psi(z) = \frac{d}{dz}\ln\Gamma(z)$,

$$\psi(z) = -C - \sum_{n=0}^{\infty}\left(\frac{1}{z+n} - \frac{1}{1+n}\right)$$

where $C = 0.577$ is the Euler constant, so that

$$\frac{1}{gN(0)} = \overbrace{\psi(\frac{1}{2}+\frac{\omega_D}{2\pi T_c})}^{\approx\ln(\omega_D/(2\pi T_c))} - \psi(\frac{1}{2}) = \ln\left(\frac{\omega_D e^{-\psi(\frac{1}{2})}}{2\pi T_c}\right),$$

We we have approximated $\psi(z) \approx \ln(z)$ for large $|z|$. Thus,

$$T_c = \overbrace{\left(\frac{e^{-\psi(1/2)}}{2\pi}\right)}^{\approx 1.13}\omega_D e^{-\frac{1}{g_0 N(0)}} \tag{14.13}$$

Notice that the details of the way we introduced the cut-off into the sums affects both the gap Δ in (14.12) and the transition temperature in (14.13). However, the ratio of twice the gap to T_C,

$$\frac{2\Delta}{T_c} = 8\pi e^{\psi(\frac{1}{2})} \approx 3.53$$

is *universal* for BCS superconductors, because the details of the cut-off cancel out of this ratio. Experiments confirm that this ratio of gap to transition is indeed observed in phonon mediated superconductors.

14.4 BCS Wavefunction and Boguilubov quasiparticles

Below the transition temperature, the finite pairing field Δ modifies the motion of the electrons. Let us examine the Hamiltonian which appears in (14.5). If restore the Grassman variables to full-fledged operators, we see that

$$\begin{aligned} H &= \sum_{\mathbf{k}} :\psi^\dagger_{\mathbf{k}} \underline{h}_{\mathbf{k}} \psi_{\mathbf{k}}: \\ &= \sum_{\mathbf{k}} :(c^\dagger_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow})\begin{bmatrix}\epsilon_{\mathbf{k}} & \Delta \\ \bar{\Delta} & -\epsilon_{\mathbf{k}}\end{bmatrix}\begin{pmatrix}c_{\mathbf{k}\uparrow}\\ \bar{c}_{-\mathbf{k}\downarrow}\end{pmatrix}: \\ &= \sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}}\left[\bar{\Delta}c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} + \Delta c^\dagger_{\mathbf{k}\uparrow}c^\dagger{}_{-\mathbf{k}\downarrow}\right] \end{aligned} \tag{14.14}$$

Notice how the off-diagonal terms associated with the pair condensate cause electrons to interconvert into holes with the same momentum and spin. This kind of scattering is sometimes referred to as "Andreev scattering"[1]. In making this transformation, charge $2e$ is transferred into the electron condensate.

One of the interesting aspects of superconductivity, is that it can be regarded as closely analogous to a magnetic ordering process. Magnetism involves an ordering or condensation of spins. Superconductivity takes place in charge rather than spin space, and we may regard the Nambu isospin operators $\vec{\tau}$ as a direct analog of the Pauli spin operators, operating in charge or "isospin" space.

It is very convenient to introduce the unit vector, defined by

$$\hat{n}_{\mathbf{k}} = \left(\frac{\Delta_1}{E_{\mathbf{k}}}, \frac{\Delta_2}{E_{\mathbf{k}}}, \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right)$$

where as before, $E_{\mathbf{k}} = \sqrt{\epsilon^2_{\mathbf{k}} + |\Delta|^2}$ is the energy of the paired electrons. Notice that $\hat{n}^2 = 1$ is a unit vector. For the discussion here, we shall choose the phase of Δ so that $\Delta_2 = 0$. In terms of this vector,

$$\underline{h}_{\mathbf{k}} = \epsilon_{\mathbf{k}}\tau_3 + \Delta_1\tau_1 + \Delta_2\tau_2 = E_{\mathbf{k}}\hat{n}_{\mathbf{k}}\cdot\vec{\tau}$$

[1] Andreev noticed that although the momentum of the hole is the same as the incoming electron, its group velocity $\nabla_{\mathbf{k}}(-\epsilon_{-\mathbf{k}}) = \nabla_{\mathbf{k}}(-\epsilon_{\mathbf{k}}) = -\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}$, is reversed. Andreev reasoned that such scattering at the interface of a superconductor leads to non-specular reflection of electrons, which scatter back as holes movign in the opposite direction to incoming electrons.

where $\vec{\tau} = (\tau_1, \tau_2, \tau_3)$. The vector $\hat{n}$ points "upwards" above the Fermi surface, and "downwards" beneath it. In a normal metal, the $\hat{n}$ vector abruptly reverses at the Fermi surface forming a sharp domain wall. In a superconductor, the $\hat{n}$ vector is aligned at an angle θ to the $\hat{z}$ axis, where

$$\cos\theta = \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}},$$

and the domain wall is now spread out over a kinetic energy range of order Δ, as shown in figure (14.1). From this perspective, $\vec{B}_{\mathbf{k}} = -E_{\mathbf{k}}\hat{n}_{\mathbf{k}}$ is a kind of "Weiss field" acting in isopsin space. This

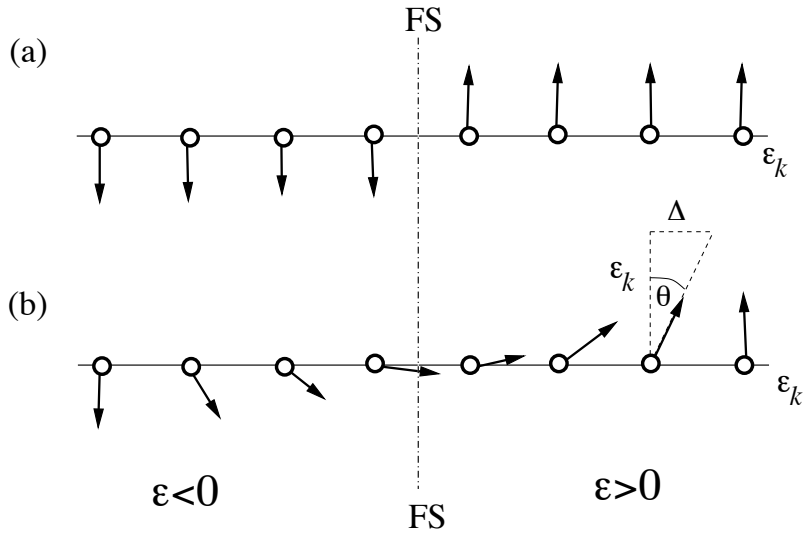


Figure 14.1: Showing the reversal of the isospin direction $\hat{n}$ around the Fermi momentum for (a) a normal metal and (b) a superconductor.

is the basis of Anderson's "pseudo-spin" interpretation of the BCS ground-state. According to this picture, one expects the isospin at each momentum $\mathbf{k}$ to align itself parallel to this field, i.e

$$\langle \psi^\dagger_{\mathbf{k}} \vec{\tau} \psi_{\mathbf{k}} \rangle = -\hat{n}_{\mathbf{k}} = -(\sin\theta_{\mathbf{k}}, 0, \cos\theta_{\mathbf{k}})$$

In a normal metal, the "z" component of the isospin is given by

$$\psi^\dagger_{\mathbf{k}} \tau_3 \psi_{\mathbf{k}} = n_{\mathbf{k}\uparrow} + n_{\mathbf{k}\downarrow} - 1 = \begin{cases} -1 & (k > k_F) \\ 1 & (k < k_F) \end{cases}$$

but in a superconductor, this becomes

$$2n_{\mathbf{k}} - 1 = -\frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2}}$$

so the occupancy becomes smeared around the Fermi surface.

Let us begin by constructing the BCS ground-state wavefunction. We wish to construct a state where the isospin at each k vector is rotated to be antiparallel to the effective field $\vec{B}_{\mathbf{k}} = -E_{\mathbf{k}}\hat{n}_{\mathbf{k}}$. At each k vector, we shall identify the empty state and doubly occupied state as "down" and "up" states respectively:

$$\begin{aligned} |\Downarrow_{\mathbf{k}}\rangle &\equiv |n_{\mathbf{k}} = 0\rangle \\ |\Uparrow_{\mathbf{k}}\rangle &\equiv |n_{\mathbf{k}} = 2\rangle = c^\dagger{}_{\mathbf{k}\uparrow} c^\dagger{}_{-\mathbf{k}\downarrow}|0\rangle. \end{aligned} \tag{14.15}$$

To produce the state where the isospin is rotated through an angle $\theta_{\mathbf{k}}$ about the y axis, we act on the vacuum with the isospin rotation operator as follows

$$\begin{aligned} |\theta_{\mathbf{k}}\rangle = e^{-i\frac{\theta_{\mathbf{k}}}{2}\psi^\dagger{}_{\mathbf{k}}\tau_y\psi_{\mathbf{k}}}|\Downarrow_{\mathbf{k}}\rangle &= \Big(\cos\frac{\theta_{\mathbf{k}}}{2} - i\sin\frac{\theta_{\mathbf{k}}}{2}\psi^\dagger{}_{\mathbf{k}}\tau_y\psi_{\mathbf{k}}\Big)|\Downarrow_{\mathbf{k}}\rangle \\ &= \cos\frac{\theta_{\mathbf{k}}}{2}|\Downarrow_{\mathbf{k}}\rangle - \sin\frac{\theta_{\mathbf{k}}}{2}|\Uparrow_{\mathbf{k}}\rangle \\ &= \Big(\cos\frac{\theta_{\mathbf{k}}}{2} - \sin\frac{\theta_{\mathbf{k}}}{2}c^\dagger{}_{\mathbf{k}\uparrow}c^\dagger{}_{-\mathbf{k}\downarrow}\Big)|\Downarrow_{\mathbf{k}}\rangle \end{aligned} \tag{14.16}$$

The ground-state will then be a product of these isospin states

$$|BCS\rangle = \prod_{\mathbf{k}} |\theta_{\mathbf{k}}\rangle = \prod_{\mathbf{k}} \Big(\cos\frac{\theta_{\mathbf{k}}}{2} - \sin\frac{\theta_{\mathbf{k}}}{2}c^\dagger{}_{\mathbf{k}\uparrow}c^\dagger{}_{-\mathbf{k}\downarrow}\Big)|0\rangle \tag{14.17}$$

By convention, the coefficients $\cos\left(\frac{\theta_{\mathbf{k}}}{2}\right)$ and $\sin\left(\frac{\theta_{\mathbf{k}}}{2}\right)$ are labelled $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ respectively, where, writing

$$\begin{aligned} u^2_{\mathbf{k}} \equiv \cos^2\left(\frac{\theta_{\mathbf{k}}}{2}\right) &= \frac{1}{2}\Big[1 + \overbrace{\cos\theta_{\mathbf{k}}}^{\frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}}\Big] = \frac{1}{2}\Big[1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\Big] \\ v^2_{\mathbf{k}} \equiv \sin^2\left(\frac{\theta_{\mathbf{k}}}{2}\right) &= \frac{1}{2}\Big[1 - \cos\theta_{\mathbf{k}}\Big] = \frac{1}{2}\Big[1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\Big] \end{aligned} \tag{14.18}$$

By convention, the normalization of this state is dropped, and the BCS wavefunction is written

$$|BCS\rangle = \prod_{\mathbf{k}} |\theta_{\mathbf{k}}\rangle = \prod_{\mathbf{k}} \big(1 + \gamma_{\mathbf{k}} c^\dagger{}_{-\mathbf{k}\downarrow} c^\dagger{}_{\mathbf{k}\uparrow}\big)|0\rangle, \qquad (\gamma_{\mathbf{k}} = \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}}) \tag{14.19}$$

Remarks

- Since $(c^\dagger_{-\mathbf{k}\downarrow}c^\dagger_{\mathbf{k}\uparrow})^2 = 1, (1+\gamma_{\mathbf{k}}c^\dagger_{-\mathbf{k}\downarrow}c^\dagger_{\mathbf{k}\uparrow}) = Exp(\gamma_{\mathbf{k}}c^\dagger_{-\mathbf{k}\downarrow}c^\dagger_{\mathbf{k}\uparrow})$, the BCS wavefunction can be re-written as an explicit coherent state

$$|BCS\rangle = e^{b^\dagger}|0\rangle$$

where

$$b^\dagger = \sum_{\mathbf{k}} \gamma_{\mathbf{k}} c^\dagger_{-\mathbf{k}\downarrow} c^\dagger_{\mathbf{k}\uparrow}$$

is the bosonic pair operator that condenses.

- The BCS ground-state has an indefinite number of particles and can be written as a linear combination of states of definite numbers of particles

$$|BCS\rangle = \sum \frac{1}{n!}|n\rangle$$

where $|n\rangle = (b^\dagger)^n|0\rangle$ is a state of n electron pairs. Since the pair operator has condensed, it costs no energy to add a pair, and in the thermodynamic limit, each of these states has the same free energy per unit volume.

- If the phase of the electron operator is changed $c^\dagger_{\mathbf{k}\sigma} \to e^{i\theta}c^\dagger_{\mathbf{k}\sigma}$, the pair order parameter $\Delta = -g\sum_{\mathbf{k}}\langle c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle$, until now assumed to be real, acquires a phase $\Delta \to e^{-2i\theta}\Delta$, and the BCS wavefunction becomes

$$|\theta\rangle = \prod_{\mathbf{k}} |\theta_{\mathbf{k}}\rangle = \prod_{\mathbf{k}} \left(1 + e^{i2\theta}\gamma_{\mathbf{k}}c^\dagger_{-\mathbf{k}\downarrow}c^\dagger_{\mathbf{k}\uparrow}\right)|0\rangle = \sum \frac{1}{n!}e^{i2n\theta}|n\rangle \qquad (14.20)$$

The action of the number operator $\hat{N}$ on this state may be represented as a differential with respect to phase,

$$\hat{N}|\theta\rangle = \sum \frac{1}{n!}2ne^{i2n\theta}|n\rangle = -i\frac{d}{d\theta}|\theta\rangle.$$

so that

$$\hat{N} \equiv -i\frac{d}{d\theta}.$$

In other words, the phase of the order parameter is conjugate to the number operator, and like position and momentum, or energy and time, the two variables therefore obey an uncertainty principle

$$\Delta\theta\Delta N \gtrsim 1.$$

so that a state of matter with a precise phase, has an ill-defined particle number.

- The electron pair operator $b^\dagger$ can also be rewritten as a real-space operator

$$b^\dagger = \int d^3r \int d^3r' \gamma(\vec{r}-\vec{r}')\psi^\dagger{}_\downarrow(\vec{r})\psi^\dagger{}_\uparrow(\vec{r}')$$

where $\gamma(\vec{r})$is the Fourier transform of $\gamma_{\mathbf{k}}$. In this way, we see that $b^\dagger$ creates a single Cooper pair with a spatial wavefunction given by $\gamma(\vec{x}-\vec{x}')$. The spatial extent of the Cooper pair is governed by the region of momentum space where $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ deviate significantly from unity or zero - i.e the area within a momentum Δk_F of the Fermi surface, where $v_F\Delta k \lesssim \Delta$. The corresponding spatial extent of the Cooper pair is then

$$\xi \sim \frac{1}{\Delta k} = \frac{v_F}{\Delta}$$

This length is known as the "coherence length" of a superconductor. Notice how the larger the gap, the smaller the coherence length. Conventional superconductors have coherence lengths of several hundreds of Angstroms, but high temperature superconductors, which have very large gaps, and in heavy electron superconductors, which have very small Fermi velocities, the coherence length can drop to a size comparable with the lattice constant.

Let us now construct the quasiparticle operators that diagonalize the mean-field Hamiltonian for the paired superconductor. In a superconductor, the Andreev scattering mixes particle and holes to produce the gapped spectrum illustrated in Fig. 14.2. We accordingly expect that the quasiparticle operators are linear combinations of electron and hole states.

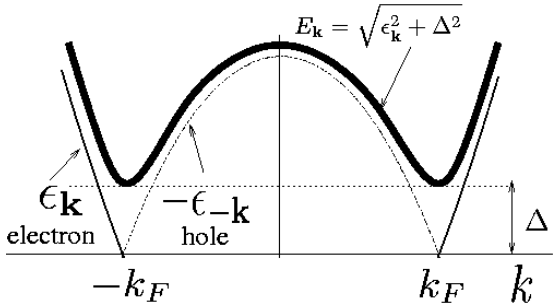


Figure 14.2: In a superconductor, the presence of the pair condensate Andreev scatters particles into holes, producing a gap in the quasiparticle excitation spectrum

Let us first recall that for any one-particle Hamiltonian $H = \psi^\dagger{}_\alpha h_{\alpha\beta}\psi_\beta$, we can construct "quasiparticle" operators $a^\dagger{}_\lambda = \psi^\dagger{}_\beta\langle\beta|\lambda\rangle$ which transform H into the diagonal form $H = \sum_\lambda E_\lambda a^\dagger{}_\lambda a_\lambda$. Now the matrix element between the original one particle state $|\alpha\rangle = \psi^\dagger{}_\alpha|0\rangle$ and the quasiparticle state $|\lambda\rangle = a^\dagger{}_\lambda|0\rangle$ is $\langle\alpha|\hat{H}|\lambda\rangle = h_{\alpha\beta}\langle\beta|\lambda\rangle == E_\lambda\langle\alpha|\lambda\rangle$, in other words, $\langle\beta|\lambda\rangle$ is an eigenvector of $h_{\alpha\beta}$. Now in BCS theory, the $\psi^\dagger{}_\alpha \equiv (c^\dagger_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow})$ are the components of the Nambu spinor, whose first and second components respectively create a particle and and a hole. Remarkably then, the procedure of diagonalizing the one-particle Hamiltonian must mix particle and hole.

To construct the quasiparticles, we note that the Nambu Hamiltonian,

$$\underline{h}_{\mathbf{k}} = E_{\mathbf{k}}\hat{n}\cdot\vec{\tau}$$

has two eigenvalues, $\pm E_{\mathbf{k}}$ with eigenvectors $\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}}\end{pmatrix}$ and $\begin{pmatrix} -v_{\mathbf{k}} \\ u_{\mathbf{k}}\end{pmatrix}$ which describe isospins that are parallel and antiparallel to $\hat{n}$, respectively. These satisfy

$$\hat{n}\cdot\vec{\tau}\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}}\end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}}\end{pmatrix}, \qquad \hat{n}\cdot\vec{\tau}\begin{pmatrix} -v_{\mathbf{k}} \\ u_{\mathbf{k}}\end{pmatrix} = -\begin{pmatrix} -v_{\mathbf{k}} \\ u_{\mathbf{k}}\end{pmatrix}$$

It follows that the appropriate quasiparticle operators for the BCS Hamiltonian are

$$\begin{aligned} \alpha^\dagger_{\mathbf{k}\uparrow} &= \psi^\dagger_{\mathbf{k}}\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}}\end{pmatrix} = c^\dagger_{\mathbf{k}\uparrow}u_{\mathbf{k}} + c_{-\mathbf{k}\downarrow}v_{\mathbf{k}} \qquad \text{Boguilubov quasiparticles} \\ \alpha_{-\mathbf{k}\downarrow} &= \psi^\dagger_{\mathbf{k}}\begin{pmatrix} -v_{\mathbf{k}} \\ u_{\mathbf{k}}\end{pmatrix} = c_{-\mathbf{k}\downarrow}u_{\mathbf{k}} - c^\dagger_{\mathbf{k}\uparrow}v_{\mathbf{k}} \end{aligned} \qquad (14.21)$$

which respectively create a spin up quasiparticle and quasihole with momentum $\mathbf{k}$. The transformation that mixes particle and hole in this way is called a Boguilubov transformation. Boguilubov originally studied this kind of transformation for interacting bosons inside a Bose-Einstein condensate.

We can combine these two quasiparticle operators into a single Nambu spinor $\alpha^\dagger{}_{\mathbf{k}}$ as follows

$$\alpha^\dagger{}_{\mathbf{k}} = (\alpha^\dagger_{\mathbf{k}\uparrow}, \alpha_{-\mathbf{k}\downarrow}) = \psi^\dagger{}_{\mathbf{k}}\overbrace{\begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}} \\ v_{\mathbf{k}} & u_{\mathbf{k}}\end{pmatrix}}^{=U_{\mathbf{k}}} = \psi^\dagger{}_{\mathbf{k}}U_{\mathbf{k}}$$

where $U_{\mathbf{k}}$ is a unitary matrix whose columns are the eigenvectors of $h_{\mathbf{k}}$. Taking the Hermitian conjugate, $\alpha_{\mathbf{k}} = U^\dagger{}_{\mathbf{k}}\psi_{\mathbf{k}}$ and since $UU^\dagger = 1$, it follows that $\psi_{\mathbf{k}} = U_{\mathbf{k}}\alpha_{\mathbf{k}}$. Now since $U_{\mathbf{k}}$ contains the eigenvectors of $h_{\mathbf{k}}$,

$$h_{\mathbf{k}}\psi_{\mathbf{k}} = \overbrace{h_{\mathbf{k}}U_{\mathbf{k}}}^{U_{\mathbf{k}}E_{\mathbf{k}}\tau_3}\alpha_{\mathbf{k}} = U_{\mathbf{k}}E_{\mathbf{k}}\tau_3\alpha_{\mathbf{k}}$$

so that

$$H = \sum_{\mathbf{k}}\psi^\dagger{}_{\mathbf{k}}\underline{h}_{\mathbf{k}}\psi_{\mathbf{k}} = \sum_{\mathbf{k}}\alpha^\dagger{}_{\mathbf{k}}E_{\mathbf{k}}\tau_3\alpha_{\mathbf{k}}$$

is diagonal in the quasiparticle basis. Written out explicitly,

$$\begin{aligned} H &= \sum_{\mathbf{k}}E_{\mathbf{k}}(\alpha^\dagger{}_{\mathbf{k}\uparrow}\alpha_{\mathbf{k}\uparrow} - \alpha_{-\mathbf{k}\downarrow}\alpha^\dagger{}_{-\mathbf{k}\downarrow}) \\ &= \sum_{\mathbf{k}\sigma}E_{\mathbf{k}}(\alpha^\dagger{}_{\mathbf{k}\sigma}\alpha_{\mathbf{k}\sigma}) - \sum_{\mathbf{k}}E_{\mathbf{k}} \end{aligned} \qquad (14.22)$$

from which we see that the ground-state energy is given by

$$E_g = -\sum_{\mathbf{k}}E_{\mathbf{k}}$$

Let us now explicitly check our results by verifying that the destruction operators $\alpha_{\mathbf{k}\sigma}$ annihilate the BCS ground-state, $\alpha_{\mathbf{k}\sigma}|BCS\rangle = 0$ To see this, first note that $\alpha_{\mathbf{k}\uparrow}$ commutes with $(u_{\mathbf{k}'} + v_{\mathbf{k}'}c^\dagger{}_{-\mathbf{k}'\downarrow}c^\dagger{}_{\mathbf{k}'\uparrow})$ unless $\mathbf{k}' = \mathbf{k}$, and in this case,

$$\begin{aligned} \alpha_{\mathbf{k}\uparrow}(u_{\mathbf{k}} + v_{\mathbf{k}}c^\dagger{}_{-\mathbf{k}\downarrow}c^\dagger{}_{\mathbf{k}\uparrow}) &= (u_{\mathbf{k}} + v_{\mathbf{k}}c^\dagger{}_{-\mathbf{k}\uparrow}c^\dagger{}_{\mathbf{k}\uparrow})\alpha_{\mathbf{k}\uparrow} + v_{\mathbf{k}}\overbrace{[\alpha_{\mathbf{k}\uparrow}, c^\dagger{}_{-\mathbf{k}\uparrow}c^\dagger{}_{\mathbf{k}\uparrow}]}^{-u_{\mathbf{k}}c^\dagger{}_{-\mathbf{k}\uparrow}} \\ &= u_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}}c^\dagger{}_{-\mathbf{k}\uparrow}c^\dagger{}_{\mathbf{k}\uparrow})c_{\mathbf{k}\uparrow} \end{aligned} \qquad (14.23)$$

so that

$$\alpha_{\mathbf{k}\uparrow}|BCS\rangle = \alpha_{\mathbf{k}\uparrow}\prod_{\mathbf{k}'}(u_{\mathbf{k}'} + v_{\mathbf{k}'}c^\dagger{}_{-\mathbf{k}'\downarrow}c^\dagger{}_{\mathbf{k}'\uparrow})|0\rangle = u_{\mathbf{k}}\prod_{\mathbf{k}'}(u_{\mathbf{k}'} + v_{\mathbf{k}'}c^\dagger{}_{-\mathbf{k}'\downarrow}c^\dagger{}_{\mathbf{k}'\uparrow})c_{\mathbf{k}\uparrow}|0\rangle = 0$$

The down-spin case can be proved in a similar fashion.

14.5 The Nambu Greens function

To describe the propagation of electrons and this interconversion between electron and hole, we require a matrix Greens function, often called the Nambu Greens function, which is just the Greens function formed from two Nambu spinors:

$$\mathcal{G}_{\alpha\beta}(\mathbf{k},\tau) = -\langle T\psi_{\mathbf{k}\alpha}(\tau)\psi^\dagger{}_{\mathbf{k}\beta}(0)\rangle \qquad (14.24)$$

which may be written out more explicitly as

$$\begin{aligned} \mathcal{G}(\mathbf{k},\tau) &= -\left\langle T\begin{pmatrix} c_{\mathbf{k}\uparrow}(\tau) \\ \bar{c}_{-\mathbf{k}\downarrow}(\tau)\end{pmatrix}\otimes(c^\dagger{}_{\mathbf{k}\uparrow}(0), c_{-\mathbf{k}\downarrow}(0))\right\rangle \\ &= -\begin{bmatrix} \langle Tc_{\mathbf{k}\uparrow}(\tau)c^\dagger{}_{\mathbf{k}\uparrow}(0)\rangle & \langle Tc_{\mathbf{k}\uparrow}(\tau)c_{-\mathbf{k}\downarrow}(0)\rangle \\ \langle Tc^\dagger{}_{-\mathbf{k}\downarrow}(\tau)c^\dagger{}_{\mathbf{k}\uparrow}(0)\rangle & \langle Tc^\dagger{}_{-\mathbf{k}\downarrow}(\tau)c_{-\mathbf{k}\downarrow}(0)\rangle\end{bmatrix} \end{aligned} \qquad (14.25)$$

The off-diagonal elements of this propagator result from the Andreev reflection. These anomalous parts of the propagator were first discussed by Gorkov, and are written as

$$F(\mathbf{k},\tau) = -\langle Tc_{\mathbf{k}\uparrow}(\tau)c_{-\mathbf{k}\downarrow}(0)\rangle, \qquad \bar{F}(\mathbf{k},\tau) = -\langle Tc^\dagger{}_{-\mathbf{k}\downarrow}(\tau)c_{\mathbf{k}\uparrow}(0)\rangle, \qquad (14.26)$$

From our general path integral result (13.133), we note that just as in the normal metal,

$$\frac{1}{i\omega_n - \epsilon_{\mathbf{k}}} = -\int_0^\beta d\tau e^{i\omega_n\tau}\langle Tc_{\mathbf{k}\sigma}(\tau)c^\dagger{}_{\mathbf{k}\sigma}\rangle, \qquad (14.27)$$

in the matrix generalization,

$$[i\omega_n - h_{\mathbf{k}}]^{-1} = \int_0^\beta d\tau e^{i\omega_n\tau}\underline{\mathcal{G}}(\mathbf{k},\tau) \tag{14.28}$$

is the Nambu propagator in Fourier space. From (14.5), we have $\underline{h}_{\mathbf{k}} = \epsilon_{\mathbf{k}}\tau_3 + \Delta_1\tau_1 + \Delta_2\tau_2$. For simplicity, lets assume that Δ is real, so that $\Delta_2 = 0$, then

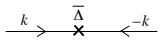
$$\underline{\mathcal{G}}(k) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}\tau_3 + \Delta\tau_1} = \frac{i\omega_n + \epsilon_{\mathbf{k}}\tau_3 + \Delta\tau_1}{(i\omega_n)^2 - E_{\mathbf{k}}^2} \tag{14.29}$$

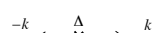
Written out explicitly, this is

$$\underline{\mathcal{G}}(\mathbf{k}, i\omega_n) = \frac{1}{(i\omega_n)^2 - E_{\mathbf{k}}^2}\begin{bmatrix} i\omega_n + \epsilon_{\mathbf{k}} & \Delta \\ \Delta & i\omega_n - \epsilon_{\mathbf{k}}\end{bmatrix} \tag{14.30}$$

where $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}$ is the quasiparticle energy. (One can restore a complex Δ by replacing $\Delta \to \bar{\Delta}$ in the lower-left component of $\underline{G}(k)$).

Let us now examine how to obtain the same results diagrammatically. The Andreev scattering converts a particle into a hole, so we we may associate scattering vertices with the Andreev reflection events as follows:

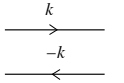
$\bar{\Delta}c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}$ ≡  $\bar{\Delta}$

$\Delta c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}$ ≡  Δ (14.31)

The "bare" propagators for the electron and hole are the diagonal components of the bare Nambu propagator

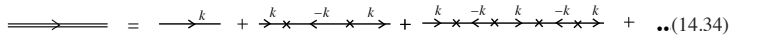
$$\underline{\mathcal{G}}_0(k) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}\tau_3} = \begin{bmatrix} \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}} & \\ & \frac{1}{i\omega_n + \epsilon_{\mathbf{k}}}\end{bmatrix}. \tag{14.32}$$

We denote these two components by the diagrams

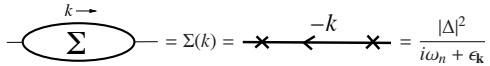
 ≡ $G_0(k) = \dfrac{1}{i\omega_n - \epsilon_{\mathbf{k}}}$

≡ $-G_0(-k) = \dfrac{1}{i\omega_n + \epsilon_{\mathbf{k}}}$ (14.33)

(The minus sign in the second term is because we have commuted creation and annihilation operators to construct the hole propagator.) The Feynman diagrams for the conventional propagator are given by

 (14.34)

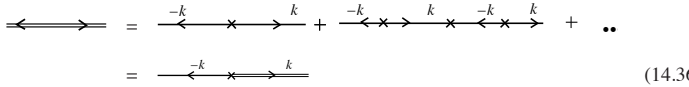
Notice how the electron Andreev scatters an even number of times. This enables us to identify a "self-energy" term that takes the form



Inserting this into the propagator, yields

$$= \frac{1}{i\omega_n - \epsilon_{\mathbf{k}} - \Sigma(i\omega_n)} = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}} - \frac{|\Delta|^2}{i\omega_n + \epsilon_{\mathbf{k}}}} = \frac{i\omega_n + \epsilon_{\mathbf{k}}}{(i\omega_n)^2 - E_{\mathbf{k}}^2}. \tag{14.35}$$

In a similar way, the anomalous propagator is given by



(14.36)

so that

$$F(k) = \frac{\Delta}{i\omega_n + \epsilon_{\mathbf{k}}}\frac{1}{i\omega_n - \epsilon_{\mathbf{k}} - \frac{|\Delta|^2}{i\omega_n + \epsilon_{\mathbf{k}}}} = \frac{\Delta}{(i\omega_n)^2 - E_{\mathbf{k}}^2}$$

Finally, note that we can also see the quasiparticle structure in the Nambu propagators. The operators

$$P_+(\mathbf{k}) = \frac{1}{2}(1 + \hat{n}\cdot\vec{\tau}), \qquad P_-(\mathbf{k}) = \frac{1}{2}(1 - \hat{n}\cdot\vec{\tau}),$$

satisfy $P_+^2 = P_+$, $P_-^2 = P_-$ and $P_+ + P_- = 1$, and furthermore,

$$P_+(\mathbf{k})(\hat{n}_{\mathbf{k}}\cdot\vec{\tau}) = P_+(\mathbf{k}), \qquad P_-(\mathbf{k})(\hat{n}_{\mathbf{k}}\cdot\vec{\tau}) = -P_-(\mathbf{k}),$$

so that these operators conveniently project the isospin onto the directions $\pm n_{\mathbf{k}}$.

We can use the projectors $P_\pm(\mathbf{k})$ to project the Nambu propagator as follows

$$\begin{aligned}\underline{\mathcal{G}} &= (P_+ + P_-)\frac{1}{i\omega_n - E_{\mathbf{k}}\hat{n}\cdot\vec{\tau}} \\ &= P_+\frac{1}{i\omega_n - E_{\mathbf{k}}\hat{n}\cdot\hat{\tau}} + P_-\frac{1}{i\omega_n - E_{\mathbf{k}}\hat{n}\cdot\hat{\tau}} \\ &= P_+\frac{1}{i\omega_n - E_{\mathbf{k}}} + P_-\frac{1}{i\omega_n + E_{\mathbf{k}}}\end{aligned} \tag{14.37}$$

we can interpret these two terms as the "quasiparticle" and "quasi-hole" parts of the Nambu propagator. If we explicitly expand out this expression, using

$$P_\pm = \frac{1}{2} \pm \begin{bmatrix} \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} & \frac{\Delta}{2E_{\mathbf{k}}} \\ \frac{\Delta}{2E_{\mathbf{k}}} & -\frac{\epsilon_{\mathbf{k}}}{2E_{\mathbf{k}}}\end{bmatrix}$$

we find that the diagonal part of the Green's function is given by

$$G(k) = \frac{u_{\mathbf{k}}^2}{i\omega_n - E_{\mathbf{k}}} + \frac{v_{\mathbf{k}}^2}{i\omega_n + E_{\mathbf{k}}}.$$

confirming that $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ determin the overlap between the electron and the quasiparticle and quasi-hole, respectively.

Example 14.1:

(a) Starting with the equation of motion of the Boguilubov quasiparticle, If the Boguilubov quasiparticle $\alpha^\dagger_{\mathbf{k}\uparrow} = c^\dagger_{\mathbf{k}\uparrow}u_{\mathbf{k}} + c_{-\mathbf{k}\downarrow}v_{\mathbf{k}}\alpha_{-\mathbf{k}\downarrow}$,

$$[H, \alpha^\dagger_{\mathbf{k}\uparrow}] = \frac{\partial \alpha^\dagger_{\mathbf{k}\uparrow}}{\partial \tau} = E_{\mathbf{k}}\alpha^\dagger_{\mathbf{k}\uparrow} \tag{14.38}$$

where $E_{\mathbf{k}}$ is the quasiparticle energy, explicitly show that $\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}$ must be an eigenvector of $h_{\mathbf{k}}$ that satisfies

$$\underline{h}_{\mathbf{k}}\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = \begin{pmatrix} \epsilon_{\mathbf{k}} & \Delta \\ \Delta & -\epsilon_{\mathbf{k}} \end{pmatrix}\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = E_{\mathbf{k}}\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}$$

(b) By solving the eigenvalue problem assuming the gap is real, show explicitly that

$$\begin{aligned} u^2_{\mathbf{k}} &= \frac{1}{2}\left[1 + \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2}}\right] \\ v^2_{\mathbf{k}} &= \frac{1}{2}\left[1 - \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2}}\right] \end{aligned} \tag{14.39}$$

Solution:

(a) We begin by writing

$$\alpha_{\mathbf{k}\uparrow} = \psi^\dagger_{\mathbf{k}} \cdot \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}$$

where $\psi^\dagger_{\mathbf{k}} = (c^\dagger_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow})$ is the Nambu spinor. Now since $[H,\ \psi^\dagger_{\mathbf{k}}] = \psi^\dagger_{\mathbf{k}}\ \underline{h}_{\mathbf{k}}$, it follows that

$$[H, \alpha^\dagger_{\mathbf{k}\uparrow}] = \psi^\dagger_{\mathbf{k}}\ \underline{h}_{\mathbf{k}}\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} \tag{14.40}$$

Comparing (14.38) and (14.40), we see that the spinor $\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}$ is an eigenvector of $h_{\mathbf{k}}$,

$$\underline{h}_{\mathbf{k}}\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = \begin{pmatrix} \epsilon_{\mathbf{k}} & \Delta \\ \Delta & -\epsilon_{\mathbf{k}} \end{pmatrix}\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = E_{\mathbf{k}}\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} \tag{14.41}$$

(b) Taking the determinant of the eigenvalue equation, $\det[\underline{h}_{\mathbf{k}} - E_{\mathbf{k}}\underline{1}] = E^2_{\mathbf{k}} - \epsilon^2_{\mathbf{k}} - \Delta^2$=0, and imposing the condition that $E_{\mathbf{k}} > 0$, we obtain obtain $E_{\mathbf{k}} = \sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2}$.
Expanding the eigenvalue equation (14.41) we obtain

$$\begin{aligned} (E_{\mathbf{k}} - \epsilon_{\mathbf{k}})u_{\mathbf{k}} &= \Delta v_{\mathbf{k}} \\ \Delta u_{\mathbf{k}} &= (E_{\mathbf{k}} + \epsilon_{\mathbf{k}})v_{\mathbf{k}} \end{aligned} \tag{14.42}$$

Multiplying these two equations, we obtain $(E_{\mathbf{k}} - \epsilon_{\mathbf{k}})u^2_{\mathbf{k}} = (E_{\mathbf{k}} + \epsilon_{\mathbf{k}})v^2_{\mathbf{k}}$, or $\epsilon_{\mathbf{k}}(u^2_{\mathbf{k}} + v^2_{\mathbf{k}}) = \epsilon_{\mathbf{k}} = E_{\mathbf{k}}(u^2_{\mathbf{k}} - v^2_{\mathbf{k}})$, since $u^2_{\mathbf{k}} + v^2_{\mathbf{k}} = 1$. It follows that $u^2_{\mathbf{k}} - v^2_{\mathbf{k}} = \epsilon_{\mathbf{k}}/E_{\mathbf{k}}$. Combining this with $u^2_{\mathbf{k}} + v^2_{\mathbf{k}} = 1$, we obtain the results given in (14.39).

14.6 Twisting the phase: the superfluid stiffness

One of the key features in a superconductor is the appearance of a complex order parameter, with a phase. It is the rigidity of this phase that endows the superconductor with its ability to sustain a superflow of electrons. This feature is held in common between superfluids and superconductors - and indeed, the liquid $He-3$ undergoes a pairing instability around $3mK$, involving a condensation of triplet Cooper pairs.

The feature of superconductors that makes them stand apart from their neutral counterparts, is our ability to couple to the phase of the condensate with the electromagnetic field. The important point here, is that the phase of the order parameter, and the vector potential are linked by gauge invariance. To see this, consider that the the microscopic Kinetic energy term

$$T = \int d^3x \frac{1}{2m}\psi^\dagger_\sigma(x)(-i\hbar\vec{\nabla} - e\vec{A}(x))^2\psi_\sigma(x))$$

is invariant under the gauge transformations

$$\begin{aligned} \psi_\sigma(x) &\rightarrow e^{i\alpha(x)}\psi_\sigma(x) \\ \vec{A}(x) &\rightarrow \vec{A}(x) + \frac{\hbar}{e}\vec{\nabla}\alpha(x) \end{aligned} \tag{14.43}$$

If we now consider the order parameter

$$\Psi(x) = \langle\psi_\downarrow(x)\psi_\uparrow(x)\rangle$$

we see that under a gauge transform, $\Psi(x) \rightarrow e^{i2\alpha(x)}\Psi(x)$, in other words, the phase of the order parameter $\Psi(x) = |\Psi(x)|e^{i\phi(x)}$, transforms as

$$\phi(x) \rightarrow \phi(x) + 2\alpha(x)$$

Now if the phase becomes "rigid" beneath T_c, then the overall energy of the superconductor must acquire a phase stiffness term of the form

$$\mathcal{F} \sim \int_x \frac{\rho_s}{2}(\nabla\phi)^2 \tag{14.44}$$

However, such a coupling term is not gauge invariant under the combined transformation

$$\begin{aligned} \phi &\rightarrow \phi + 2\alpha, \\ \vec{A} &\rightarrow \vec{A} + \frac{\hbar}{e}\vec{\nabla}\alpha(x) \end{aligned} \tag{14.45}$$

Indeed, in order that the Free energy gauge invariant, the phase stiffness must take the form

$$\begin{aligned} \mathcal{F} &\sim \int_x \frac{\rho_s}{2}\left(\vec{\nabla}\phi(x) - \frac{2e}{\hbar}\vec{A}(x)\right)^2 + \mathcal{F}_{em}[A] \\ &= \int_x \frac{Q}{2}\left(\vec{A}(x) - \frac{\hbar}{2e}\vec{\nabla}\phi(x)\right)^2 + \mathcal{F}_{em}[A] \end{aligned} \tag{14.46}$$

where $\mathcal{F}_{em}[A]$ is the Free energy of the electromagnetic field and we have substituted

$$Q = \frac{(2e)^2}{\hbar^2}\rho_s$$

Since $\mathcal{F}_{em}$ is invariant under gauge transformations, it becomes possible to redefine the vector potential

$$A(x) \to \vec{A}(x) - \frac{\hbar}{2e}\vec{\nabla}\phi(x)$$

to "absorb" the phase of the order parameter. Once the phase of the order parameter is absorbed into the electromagnetic field,

$$\mathcal{F} \sim \int_x \frac{4e^2\rho_s}{2\hbar^2}\vec{A}(x)^2 + \mathcal{F}_{em}[A], \tag{14.47}$$

and the vector potential has acquired a mass. This phenomenon whereby the gauge field, "eats up" the phase of a condensate, losing manifest gauge invariance by acquiring a mass is called the "Anderson-Higgs" mechanism. This is the root mechanism by which gauge fields acquire a mass in particle physics.

Shortly after the importance of this mechanism for relativistic Yang Mills theories was noted by Higgs and Anderson, Weinberg and Salem independently applied the idea to develop the theory of "electro-weak" interactions. According to this picture, the universe we live is a kind of cosmological Meissner phase, formed in the early universe, which excludes the weak force by making the vector bosons which carry it, become massive. It is a remarkable thought that the very same mechanism that causes superconductors to levitate lies at the heart of the weak nuclear force responsible for nuclear fusion inside stars. In trying to discover the Higg's particle, physicists are in effect trying to probe the cosmic superconductor above its gap energy scale.

If we now look back at (14.46), we see that the electrical current carried by the condensate is

$$\vec{j} = -\frac{\delta\mathcal{F}}{\delta\vec{A}(x)} = -Q\left(\vec{A}(x) - \frac{\hbar}{2e}\vec{\nabla}\phi(x)\right).$$

This permits us to identify Q with the "London Kernel" introduced earlier in the study of electron transport. What is different here, is that this quantity is now finite in the DC, zero frequency limit. Thus, once a charged order parameter develops a rigidity, the matter becomes a perfect diamagnet, developing superconductivity.

Let us now continue to calculate the phase stiffness or "superfluid density" of a BCS superconductor. Formally, to twist the phase of the order parameter, we need to allow the order parameter to become a function of position, so that now the interaction that gives rise to superconductivity can not be infinitely long-ranged. In the simplest case, we can simply consider a local interaction

$$H_I = -g\int d^3x \psi^\dagger{}_\uparrow(x)\psi^\dagger{}_\downarrow(x)\psi_\downarrow(x)\psi_\uparrow(x)$$

Under the Hubbard Stratonovich transformation, this becomes

$$H_I \to \int d^3x\left[\bar{\Delta}(x)\psi_\downarrow(x)\psi_\uparrow(x) + \psi^\dagger{}_\uparrow(x)\psi^\dagger{}_\downarrow(x)\Delta(x) + \frac{\bar{\Delta}(x)\Delta(x)}{g}\right]$$

so that now, the phase of the order parameter can develop a non-uniform configuration. We'll imagine a superconductor on a torus in which the phase of the order parameter is twisted, so that $\Delta(L) = e^{i\Delta\phi}\Delta(0)$. Let us consider a uniform twist, so that

$$\Delta(x) = e^{i\vec{a}\cdot\vec{x}}\Delta_0,$$

where $\vec{a} = \frac{\Delta\phi}{L}\hat{x}$. Now by gauge invariance, this twist of the order parameter can be removed by a gauge transformation,

$$\begin{aligned}\Delta(x) &\to e^{-i\vec{a}\cdot\vec{x}}\Delta(x) = \Delta_0\\ \vec{A} &= \vec{A} - \frac{\hbar}{2e}\vec{a}\end{aligned} \tag{14.48}$$

so a twist in the order parameter is gauge equivalent to a uniform vector potential $\vec{A} = \frac{\hbar}{2e}\vec{a}$, and vice versa- a uniform vector potential is gauge equivalent to a twisted order parameter field.

So to calculate the stiffness we need to compute the Free energy in the presence of a uniform vector potential. On a taurus, this implies a threaded magnetic flux. Indeed, the total change in the phase of the order paramter is given by

$$\Delta\phi = \alpha L = \frac{2e}{\hbar}AL = \frac{2e}{\hbar}\Phi = 2\pi\left(\frac{\Phi}{\frac{\hbar}{2e}}\right)$$

where Φ is the magnetic flux through the torus. The twist angle can by written

$$\Delta\phi = 2\pi\frac{\Phi}{\Phi_0},$$

where

$$\Phi_0 = \frac{\hbar}{2e}$$

is known as the superconducting flux quantum. Each time the flux through the taurus increases by Φ_0, the superconducting order parameter is twisted by an additional 2π.

Introduction of vector potential $\epsilon_{\vec{k}} \to \epsilon_{\vec{k}-e\vec{A}}$, so inside $h_{\mathbf{k}}$

$$\epsilon_{\vec{k}}\tau_3 \to \begin{pmatrix}\epsilon_{\vec{k}-e\vec{A}} & \\ & -\epsilon_{-\vec{k}-e\vec{A}}\end{pmatrix} = \begin{pmatrix}\epsilon_{\vec{k}-e\vec{A}} & \\ & -\epsilon_{\vec{k}+e\vec{A}}\end{pmatrix} \equiv \epsilon_{\vec{k}-e\vec{A}}\tau_3 \tag{14.49}$$

i.e ,

$$\underline{h_{\vec{k}}} \to \underline{h}_{\vec{k}-e\vec{A}\tau_3} = \epsilon_{\vec{k}-e\vec{A}\tau_3}\tau + \Delta\tau_1$$

The Free energy in a field is then

$$F = -T\sum_{\mathbf{k},i\omega_n}\mathrm{Tr}\ln[\epsilon_{\vec{k}-e\vec{A}\tau_3}\tau + \Delta\tau_1 - i\omega_n] + \frac{\Delta^2}{g}$$

We need to calculate

$$Q_{ab} = -\frac{1}{V}\frac{\partial^2 F}{\partial A_a \partial A_b}$$

Taking the first derivative with respect to the vector potential gives us the steady-state diamagnetic current

$$-\langle J_a\rangle = \frac{1}{V}\frac{\partial F}{\partial A_a} = -\frac{1}{\beta V}\sum_{k\equiv(\mathbf{k},i\omega_n)} \mathrm{Tr}\Big[e\nabla_a\epsilon_{\vec{k}-e\vec{A}\tau_3}\, G(k-eA)\Big]$$

where we have introduced the shorthand $G(k-eA) = [i\omega_n - \underline{h}_{\vec{k}-e\vec{A}\tau_3}]^{-1} = [i\omega_n - \epsilon_{\vec{k}-e\vec{A}\tau_3}\tau_3 - \Delta\tau_1]^{-1}$.

Taking one more derivative,

$$Q_{ab} = \frac{1}{V}\frac{\partial^2 F}{\partial A_a \partial A_b}\Big|_{A=0} = \frac{e^2}{\beta V}\sum_k \left(\overbrace{\nabla^2_{ab}\epsilon_{\vec{k}}\mathrm{Tr}\,[\tau_3 G(k)]}^{\text{diamagnetic part}} + \overbrace{\nabla_a\epsilon_{\vec{k}}\nabla_b\epsilon_{\vec{k}}\mathrm{Tr}\,[G(k)G(k)]}^{\text{paramagnetic part}}\right)$$

where we first used the relation $\frac{\partial}{\partial A_b}G(k-eA) = e\nabla_b\epsilon_{\vec{k}}G(k-eA)^2$ and then set $A=0$. We may identify the above expression as a sum of the diamagnetic, and paramagnetic parts, respectively, of the superfluid stiffness. The diamagnetic part of the response can be integrated by parts, to give

$$\begin{aligned}\frac{e^2}{\beta V}\sum_{\mathbf{k},n}\nabla^2_{ab}\epsilon_{\vec{k}}\mathrm{Tr}\,[\tau_3 G(k)] &= -\frac{e^2}{\beta V}\sum_{\mathbf{k},n}\nabla_a\epsilon_{\vec{k}}\mathrm{Tr}\,[\tau_3\nabla_b G(k)]\\ &= -\frac{e^2}{\beta V}\sum_{\mathbf{k},n}\nabla_a\epsilon_{\vec{k}}\nabla_b\epsilon_{\vec{k}}\mathrm{Tr}\,[\tau_3 G(k)\tau_3 G(k)]\end{aligned} \qquad (14.50)$$

Notice how this term is identical to the paramagnetic term, apart from the τ_3 insertions. We now add these two terms, to obtain

$$Q_{ab} = -\frac{e^2}{\beta V}\sum_k \nabla_a\epsilon_{\vec{k}}\nabla_b\epsilon_{\vec{k}}\left(\overbrace{\mathrm{Tr}\,[\tau_3 G(k)\tau_3 G(k)]}^{\text{diamagnetic part}} - \overbrace{\mathrm{Tr}\,[G(k)G(k)]}^{\text{paramagnetic part}}\right).$$

Notice, that when pairing is absent, the τ_3 commute with $\mathcal{G}(k)$, and the diamagnetic and paramagnetic contributions exactly cancel. We can make this explicit, by writing

$$Q_{ab} = -\frac{e^2}{2\beta V}\sum_k \nabla_a\epsilon_{\vec{k}}\nabla_b\epsilon_{\vec{k}}\mathrm{Tr}\Big[[\tau_3, G(k)]^2\Big].$$

Now

$$[\tau_3, G(k)] = 2i\frac{\Delta\tau_2}{(i\omega_n)^2 - E^2_{\mathbf{k}}}$$

so

$$-\mathrm{Tr}\Big[[\tau_3, G(k)]^2\Big] = 8\frac{\Delta^2}{[(\omega_n)^2 + \epsilon^2_{\mathbf{k}} + \Delta^2]^2}.$$

so that

$$Q_{ab} = \frac{4e^2}{\beta V}\sum_k \nabla_a\epsilon_{\vec{k}}\nabla_b\epsilon_{\vec{k}}\frac{\Delta^2}{[(\omega_n)^2 + \epsilon^2_{\mathbf{k}} + \Delta^2]^2}.. \qquad (14.51)$$

Remarkably, although the diamagnetic and paramagnetic parts of the superfluid stiffness involve electrons far away from the Fermi surface, the difference between the two is dominated by electrons near the Fermi surface. This enables us to replace

$$\frac{2}{V}\sum_{\mathbf{k}}\nabla_a\epsilon_{\vec{k}}\nabla_b\epsilon_{\vec{k}}\{\ldots\} = N(0)\int_{-\infty}^{\infty}d\epsilon\int\overbrace{\frac{d\Omega_{\hat{\mathbf{k}}}}{4\pi}v_a v_b}^{\frac{1}{3}v_F^2\delta_{ab}}\{\ldots\} = \frac{\delta_{ab}}{3}N(0)v_F^2\int_{-\infty}^{\infty}d\epsilon\,\{\ldots\}.$$

Note that the factor of two is absorbed into the total density of states of up and down electrons. We have taken advantage of the rapid convergence of the integrand to extend the limits of the integral over energy to infinity. Replacing $\frac{1}{3}N(0)v_F^2 = \frac{n}{m}$, we can now write $Q_{ab} = Q\delta_{ab}$, where

$$Q(T) = \frac{ne^2}{m}T\sum_n\int_{-\infty}^{\infty}d\epsilon\frac{2\Delta^2}{(\epsilon^2+\omega_n^2+\Delta^2)^2} = \left(\frac{ne^2}{m}\right)\pi T\sum_n\frac{\Delta^2}{(\omega_n^2+\Delta^2)^{\frac{3}{2}}}$$

To evaluate this expression, it is useful to note that the argument of the summation is a total derivative so that

$$Q(T) = \left(\frac{ne^2}{m}\right)\pi T\sum_n\frac{\partial}{\partial\omega_n}\left(\frac{\omega_n}{(\omega_n^2+\Delta^2)^{1/2}}\right)$$

Now at absolute zero, we can replace $T\sum_n \to \int\frac{d\omega}{2\pi}$, so that

$$Q(0)\equiv Q_0 = \left(\frac{ne^2}{m}\right)\overbrace{\int_{-\infty}^{\infty}\frac{d\omega}{2}\frac{d}{d\omega}\left(\frac{\omega}{(\omega^2+\Delta^2)^{1/2}}\right)}^{=1} = \left(\frac{ne^2}{m}\right).$$

In other words, all of the electrons have condensed to form a perfect diamagnet. To evaluate the stiffness at a finite temperature, we rewrite the Matsubara sum as a clockwise contour integral around the poles of the Fermi function

$$Q(T) = \pi Q_0\oint_{\text{Im axis}}\frac{dz}{2\pi i}f(z)\frac{d}{dz}\left(\frac{z}{\sqrt{\Delta^2-z^2}}\right) \qquad (14.52)$$

By deforming the integral to run anti-clockwise around the branch-cuts along the real axis, and then integrating by parts we obtain:

$$\begin{aligned}Q(T) &= Q_0\pi\oint_{\text{real axis}}\frac{dz}{2\pi i}f(z)\frac{d}{dz}\left(\frac{z}{\sqrt{\Delta^2-z^2}}\right)\\ &= Q_0\int_{-\infty}^{\infty}d\omega f(\omega)\frac{d}{d\omega}\mathrm{Im}\left(\frac{z}{\sqrt{\Delta^2-z^2}}\right)_{z=\omega-i\delta}\\ &= Q_0\left[f(\omega)\mathrm{Im}\left(\frac{z}{\sqrt{\Delta^2-z^2}}\right)_{z=\omega-i\delta}\right]_{-\infty}^{\infty} + Q_0\int_{-\infty}^{\infty}d\omega\left(-\frac{df(\omega)}{d\omega}\right)\mathrm{Im}\left(\frac{z}{\sqrt{\Delta^2-z^2}}\right)_{z=\omega-i\delta}\end{aligned} \qquad (14.53)$$

Now a careful calculation of the imaginary part of the integrand gives

$$\mathrm{Im}\left(\frac{\omega}{\sqrt{\Delta^2-(\omega-i\delta)^2}}\right) = \mathrm{Im}\left(\frac{\omega}{\sqrt{-(\omega^2-\Delta^2)+i\delta\,\mathrm{sgn}(\omega)}}\right) = \left(-\frac{|\omega|}{\sqrt{\omega^2-\Delta^2}}\right)\theta(\omega^2-\Delta^2) \qquad (14.54)$$

so the finite temperature stiffness can then be written

$$Q(T) = Q_0\left[1 - 2\int_{\Delta(T)}^{\infty} d\omega\left(-\frac{df(\omega)}{d\omega}\right)\left(\frac{\omega}{\sqrt{\omega^2-\Delta^2}}\right)\right] \tag{14.55}$$

where the factor of two derives from folding over the contribution from the negative region of the integral. The second term in this expression is nothing more that the thermal average of the quasiparticle density of states $N_{qp}(E) = N(0)\frac{E}{\sqrt{E^2-\Delta^2}}$. This term can thus be interpreted as the reduction in the condensate fraction due to a thermal depopulation of the condensate into quasiparticles. We can alternatively re-write this expression as a formula for the temperature dependent penetration depth

$$\frac{1}{\lambda_L^2(T)} = \frac{1}{\lambda_L^2(0)}\left[1 - 2\overline{\left(\frac{N_{qp}(E)}{N(0)}\right)}\right].$$

where $1/\lambda_L^2(0) = \frac{\mu_0 n e^2}{m}$

Bibliography

Chapter 15

Local Moments and the Kondo effect.

15.1 Strongly Correlated Electrons

One of the fascinating growth areas in condensed matter physics concerns "strongly correlated systems": states of matter in which the many body interaction energies dominate the kinetic energies, becoming large enough to qualitatively transform the macroscopic properties of the medium. Some of the growing list of strongly correlated systems include

- Cuprate superconductors, where interactions amongst electrons in localized 3d-shells form an antiferromagnetic "Mott" insulator, which develops high temperature superconductivity when doped.
- Heavy electron compounds, in which localized magnetic moments immersed within the metal give rise to electron quasiparticles with effective masses in excess of 1000 bare electron masses.
- Fractional Quantum Hall systems, where the interactions between electrons in the lowest Landau level of a two-dimensional electron fluid generate a incompressible state with quasiparticles of fractional charge and statistics.
- "Quantum Dots", which are tiny pools of electrons in semiconductors that act as artificial atoms. As the gate voltage is changed, the Coulomb repulsion between electrons in the dot leads to the a "Coulomb Blockade", whereby electrons can be added one by one to the quantum dot.
- Cold atomic gases, in which the interactions between the neutral atoms governed by two-body resonances, can be tuned by external magnetic fields to create a whole new world of strongly correlated quantum fluids.

In each case, the interactions between the particles have been tuned - by electronic or nuclear chemistry, by geometry or nanofabrication, to give rise to a state of condensed matter in which

the interactions between the particles are large compared with their typical kinetic energy. The next two chapters will introduce a corner strongly correlated electron physics: the physics of local moments and heavy fermion compounds. A large class of strongly correlated materials contain atoms with partially filled d, or f orbitals. Heavy electron materials are an extreme example, in in which one component of the electron fluid is highly localized, usually inside f-orbitals giving rise to the formation of magnetic moments. The interaction of localized magnetic moments with the conduction sea provides the driving force for the strongly correlated electron physics in these materials.

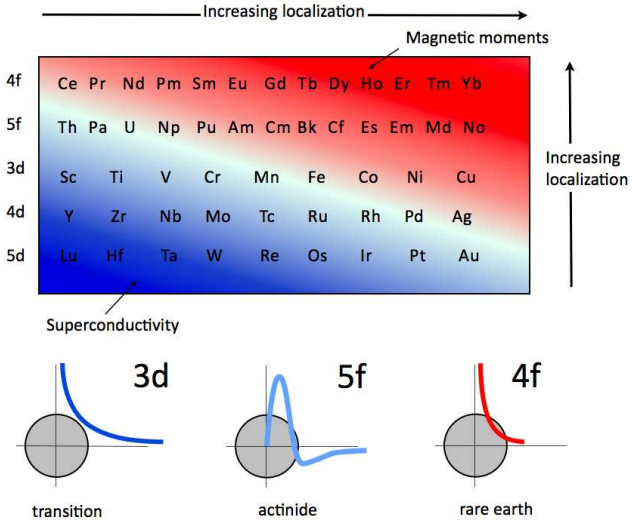


Figure 15.1: The Kmetko-Smith diagram, showing the broad trends towards increasing electron localization in the d- and f-electron compounds.

Within the periodic table, there are broad trends that govern strongly correlated electron behavior. The most strongly interacting electrons tend to reside in partially filled orbitals that are well-localized around the nucleus. The weak overlap between these orbitals and the orbitals of other nearby atoms promotes the formation of narrow electron bands, while the interactions between electrons are maximized when they occupy the same, highly localized orbital.

In order of increasing degree of localization, the unfilled electron orbitals of the central rows of the periodic table may be ordered

$$5d < 4d < 3d < 5f < 4f.$$

There are two trends operating here: first, orbitals with higher principle quantum numbers tending to be more delocalized, so that $5d < 4d < 3d$ and $5f < 4f$. Second, as we move from d to f orbitals, or along a particular row of the periodic table, the increasing nuclear charge reduces the size of the orbitals. These trends are summarized by the Kmetko-Smith diagram in Fig 15.1, in which the central rows of the periodic table are stacked in order of increasing localization. Moving up and to the right in this diagram leads to increasingly localized atoms In metals lying on the bottom-left hand side of this diagram, the d-orbitals are highly itinerant giving rise to the metals exhibit conventional superconductivity at low temperatures. By contrast, in metals towards the top right hand side of the diagram, the electrons in the rare earth or actinide ions are localized, forming magnets, or more typically, antiferromagnets.

The materials that lie in the cross-over between these two regions are particularly interesting, for these materials are "on the brink of magnetism". With some exceptions, it is in this region that the the cerium and uranium heavy fermion materials, and the iron based superconductors are found.

15.2 Local moments

To understand heavy electron materials, we need to understand how electrons form local moments, and how those local moments interact with the electrons in the conduction sea. The simplest example of a localized moment is an unpaired electron bound in an isolated atom, or ion (15.2 (a)). At temperatures far below the ionization energy $|E_f|$, the only remaining degree of freedom of this localized electron is its magnetic moment, described by the operator

$$\vec{M} = \mu_B \vec{\sigma}$$

where $\vec{\sigma}$ denotes the Pauli matrices and $\mu_B = \frac{e\hbar}{2m}$ is the Bohr magneton. In a magnetic field, the Hamiltonian describing low energy physics is simply $H = -\vec{M}\cdot\vec{B} = -\mu_B\vec{\sigma}\cdot\vec{B}$, giving rise giving rise to a "Curie" susceptibility

$$\chi(T) = \frac{\partial M}{\partial B} = -\frac{\partial^2 F}{\partial B^2} = \frac{\mu_B^2}{T}$$

The classic signature of local moments is the appearance of Curie paramagnetism with a high-temperature magnetic susceptibility of the form

$$\chi \approx n_i \frac{M^2}{3(T+\theta)} \qquad M^2 = g^2\mu_B^2 J(J+1), \tag{15.1}$$

where, n_i is the concentration of magnetic moments while M is the magnetic moment with total angular momentum quantum number J and gyro-magnetic ratio ("g-factor") g. θ is the "Curie

Weiss" temperature, a phenomenological scale which takes account of interactions between spins[1]. For a pure spin, $J = S$ is the total spin and $g = 2$, but for rare earth and actinide ions, the orbital and spin angular momentum combine into a single entity with angular momentum $\vec{J} = \vec{L} + \vec{S}$ for which g lies between one and two. For example, a Ce^{3+} ion contains a single unpaired 4f-electron in the state $4f^1$, with $l = 3$ and $s = 1/2$. Spin-orbit coupling gives rise to low-lying multiplet with $j = 3 - \frac{1}{2} = \frac{5}{2}$, consisting of $2j+1 = 6$ degenerate orbitals $|4f^1 : Jm\rangle$, $(m_J \in [-\frac{5}{2}, \frac{5}{2}])$ with an associated magnetic moment $M = 2.64\mu_B$.

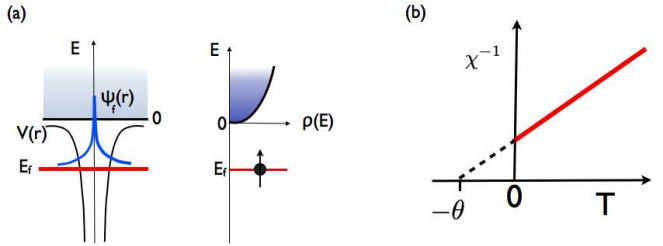


Figure 15.2: (a) In isolation, the localized atomic states of an atom form a stable, sharp excitation lying below the continuum. (b) The inverse of the Curie-Weiss susceptibility of local moments χ^{-1} is a linear function of temperature, intersecting zero at $T = -\theta$.

Though the concept of localized moments was employed in the earliest applications of quantum theory to condensed matter[2], a theoretical understanding of the *mechanism* of moment formation did not develop until the early sixties, when experimentalists began to systematically study impurities in metals. [3] In the early 1960s, Clogston, Mathias and collaborators[**?**] showed that when small concentrations n_i of magnetic ions, such as iron are added to a metallic host, they do not always form magnetic moments. For example, iron impurities in pure niobium do not develop a local moment, but they do so in the niobium-molybdenum alloy, $Nb_{1-x}Mo_x$ once the concentration of molybdeneum exceeds 40% ($x > 0.4$). It was these observations that led Anderson to develop his model for local moment formation.

[1] A positive $\theta > 0$ indicates an antiferromagnetic interaction between spins, while a negative $\theta < 0$ is associated with ferromagnetic interactions. giving rise to a divergence of the susceptibility at the Curie temperature $T_c = -\theta$.

[2] The concept of a local moment appears in Heisenberg's original paper on ferromagnetism[**?**]. Landau and Néel invoked the notion of the localized moment in their 1932 papers on antiferromagnetism, and in 1933, Kramers used this idea again in his theory of magnetic superexchange.

[3] It was not until the sixties that materials physicists could control the concentration of magnetic impurities in the parts per million range required for the study of individual impurities. The control of purity evolved during the 1950s, with the development of new techniques needed for semiconductor physics, such as zone refining.

15.3 Anderson's Model of Local Moment Formation

Anderson's model for moment formation, proposed in 1963, combines two essential ideas[**?**]:

- the localizing influence of Coulomb interactions. Peierls and Mott [**?** **?**] had reasoned in the 1940s that strong-enough Coulomb repulsion between electrons in an atomic state would blockade the passage of electrons, converting a metal into what is now called a "Mott insulator". These ideas were independently explored by Van Vleck and Hurvitz in an early attempt to understand magnetic ions in metals[**?**].
- the formation of an electronic resonance. In the 1950's Friedel and Blandin [**?** **?** **?**] proposed that electrons in the core states of magnetic atoms tunnel out into the conduction sea, forming a resonance.

Anderson unified these ideas in a second-quantized Hamiltonian

$$H = \overbrace{\sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\sigma} \left[V(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} f_\sigma + V^*(\mathbf{k}) f^\dagger_\sigma c_{\mathbf{k}\sigma} \right]}^{H_{resonance}} + \underbrace{E_f n_f + U n_{f\uparrow} n_{f\downarrow}}_{H_{atomic}}, \tag{15.2}$$

Anderson model.

where H_{atomic} describes the atomic limit of an isolated magnetic ion containing a Kramer's doublet of energy E_f. The engine of magnetism in the Anderson model is the Coulomb interaction

$$U = \frac{e^2}{4\pi\epsilon_0} \int_{\mathbf{r},\mathbf{r}'} \frac{1}{|\mathbf{r}-\mathbf{r}'|} \rho_f(\mathbf{r}) \rho_f(\mathbf{r}')$$

of a doubly occupied f-state, where $\rho_f(\mathbf{r}) = |\Psi_f(\mathbf{r})|^2$ is the electron density in a single atomic orbital $\psi_f(\mathbf{r})$. The operator $c^\dagger_{\mathbf{k}\sigma}$ creates a conduction electron of momentum $\mathbf{k}$, spin σ and energy $\epsilon_{\mathbf{k}} = E_{\mathbf{k}} - \mu$, while

$$f^\dagger_\sigma = \int_{\mathbf{r}} \Psi_f(\mathbf{r}) \hat{\psi}^\dagger_\sigma(r), \tag{15.3}$$

creates an f-electron in the atomic f-state. Unlike the electron continuum in a vacuum, a conduction band in a metal has a finite energy width, so in the model, the energies are taken lying in the range $\epsilon_{\mathbf{k}} \in [-D, D]$. $H_{resonance}$ describes the hybridization with the Bloch waves of the conduction sea that develops when the ion is immersed in a metal. The quantity

$$V(\mathbf{k}) = \langle \mathbf{k}|V_{ion}|f\rangle = \int d^3r e^{-i\mathbf{k}\cdot\mathbf{r}} V_{ion}(r) \Psi_f(\vec{r}). \tag{15.4}$$

is the hybridization between the ionic potential and a plane wave. This term is the result of applying first order perturbation theory to the degenerate states of the conduction sea and the atomic f-orbital.

A competition between localization and hybridization.

To understand the formation and properties of local moments, we need to examine the two limiting types of behaviour in the Anderson model:

- Localized moment behavior, described by the limiting case where the hybridization vanishes.
- Virtual bound-state formation, described by the limiting case where the interaction is negligible.

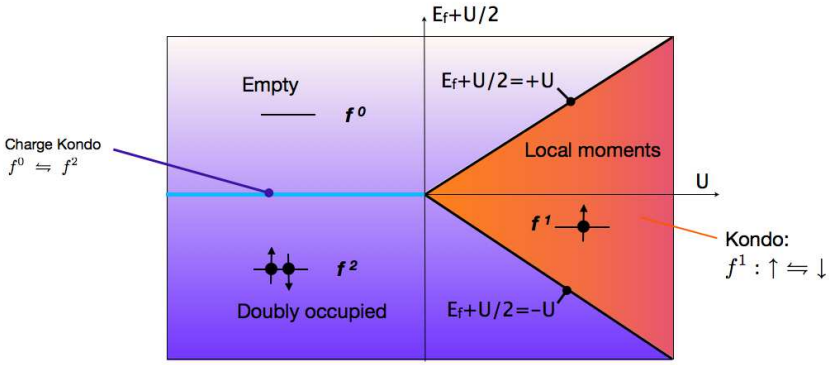


Figure 15.3: Phase diagram for Anderson impurity model in the atomic Limit. For $U > |E_f + U/2$, the ground-state is a magnetic doublet. When $U < 0$, the ground-state is degenerate charge doublet provided $E_f + U/2 = 0$.

15.3.1 The Atomic limit.

The atomic physics of an isolated ion, described by

$$H_{atomic} = E_f n_f + U n_{f\uparrow} n_{f\downarrow}. \tag{15.5}$$

is the engine at the heart of the Anderson model that drives moment formation. The four atomic quantum states are

$$\begin{array}{lll} |f^2\rangle & E(f^2) = 2E_f + U & \left.\begin{array}{l}\\ \end{array}\right\} \text{non-magnetic} \\ |f^0\rangle & E(f^0) = 0 & \\ |f^1\uparrow\rangle, \quad |f^1\downarrow\rangle & E(f^1) = E_f. & \text{magnetic.} \end{array} \tag{15.6}$$

The cost of adding or removing to the magnetic f^1 state is given by

$$\left.\begin{array}{ll} \text{adding:} & E(f^2) - E(f^1) = U + E_f \\ \text{removing:} & E(f^0) - E(f^1) = -E_f \end{array}\right\} \Rightarrow \Delta E = \frac{U}{2} \pm (E_f + \frac{U}{2}) \tag{15.7}$$

In other words, provided (Fig. 15.3)

$$U/2 > |E_f + U/2| \tag{15.8}$$

the ground-state of the atom is a two-fold degenerate magnetic doublet. Indeed, provided it is probed at energies below the smallest charge excitation energy, $\Delta E_{min} = U/2 - |E_f + U/2|$, only the spin degrees of freedom remain, and the system behaves as a local moment - a "quantum top". The interaction between such a local moment and the conduction sea gives rise to the "Kondo effect" that will be the main topic of this chapter.

Although we shall be mainly interested in positive, repulsive U, we note that in the attractive region of the phase diagram ($U < 0$) the atomic ground-state can form a degenerate "charge" doublet ($|f^0\rangle, |f^2\rangle$) or "isospin". For $U < 0$, when $E_f + U/2 = 0$ the doubly occupied state $|f^2\rangle$ and the empty state $|f^0\rangle$ become degenerate. This is the charge analog of the magnetic doublet that exists for $U > 0$, and when coupled to the sea of electrons, gives rise to an effect known as the "charge Kondo effect". Such charge doublets are thought to be important in certain "negative U" materials, such as Tl doped $PbTe$.

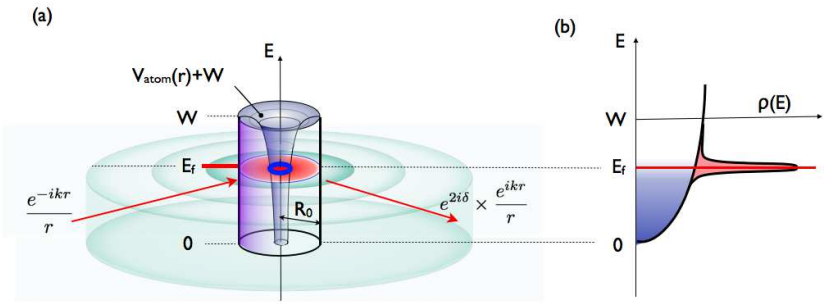


Figure 15.4: (a) The immersion of an atomic f state in a conduction sea leads to hybridization between the localized f-state and the degenerate conduction electron continuum, forming (b) a resonance in the density of states.

Example 15.1: Derivation of the non-interacting Anderson model

Consider an isolated ion, where the f-state is a solution of the one-particle Schrödinger equation

$$\left[-\nabla^2 + \hat{V}_{ion}\right]|f\rangle = E_f^{ion}|f\rangle, \tag{15.9}$$

where $V_{ion}(r)$ is the ionic potential and $E_f^{ion} < 0$ is the energy of the atomic f-level. In a metal, the positive ionic background draws the continuum downwards to become degenerate with the f-level as shown in Fig. 15.4. A convenient way to model this situation is to use "muffin tin potential", [4]

$$V(r) = (V_{ion}(r) + W)\,\theta(R_0 - r) \tag{15.10}$$

equal to the ionic potential, shifted upwards by an amount W inside the muffin tin radius R_0. The f-state is now an approximate eigenstate of $\mathcal{H} = -\nabla^2 + \hat{V}$ that is degenerate with the continuum.

Derive the non-interacting component of the Anderson model using degenerate perturbation theory, evaluating the matrix elements of $\mathcal{H}$ between the conduction states $|\mathbf{k}\rangle$ and the local f-state $|f\rangle$. You may assume that the muffin tin R_0 is much smaller than the Fermi wavelength, so that the conduction electron matrix elements $V_{\mathbf{k},\mathbf{k}'} = \langle \mathbf{k}|V|\mathbf{k}'\rangle$ are negligible.

Solution:

To carry out degenerate perturbation theory on $\mathcal{H}$ we must first orthogonalize the f-state to the continuum $|\tilde{f}\rangle = |f\rangle - \sum_{\epsilon_\mathbf{k}\in[-D,D]} |\mathbf{k}\rangle\langle\mathbf{k}|f\rangle$, where D is the conduction electron band-width. Now we need to evaluate the matrix elements of $\mathcal{H} = -\nabla^2 + V$. If we set

$$V_{\mathbf{k},\mathbf{k}'} = \int_{r<R_0} d^3r e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}(V_{ion}(r) + W), \tag{15.11}$$

then the conduction electron matrix elements are

$$\langle \mathbf{k}|\mathcal{H}|\mathbf{k}'\rangle = E_\mathbf{k}\delta_{\mathbf{k},\mathbf{k}'} + V_{\mathbf{k},\mathbf{k}'} \approx E_\mathbf{k}\delta_{\mathbf{k},\mathbf{k}'} \tag{15.12}$$

while $\langle \tilde{f}|\mathcal{H}|\tilde{f}\rangle \approx E_f^{ion}$ is the f-level energy.

The hybridization is given by the off-diagonal matrix element,

$$V(\mathbf{k}) = \langle \mathbf{k}|\mathcal{H}|\widetilde{f}\rangle = \langle \mathbf{k}| - \nabla^2 + \hat{V}|\widetilde{f}\rangle = E_\mathbf{k}\langle \mathbf{k}|\widetilde{f}\rangle + \langle \mathbf{k}|\hat{V}|\widetilde{f}\rangle = \langle \mathbf{k}|\hat{V}|\widetilde{f}\rangle, \tag{15.13}$$

where we have used the orthogonality $\langle \mathbf{k}|\tilde{f}\rangle = 0$ to eliminate the kinetic energy. Infact, since the f-state is highly localized, its overlap with the conduction electron states is small $\langle \mathbf{k}|f\rangle \approx 0$, so we can now drop the tilde, approximating $\langle \mathbf{k}|\hat{V}|\widetilde{f}\rangle \approx \langle \mathbf{k}|\hat{V}_{ion} + W|f\rangle \approx \langle \mathbf{k}|\hat{V}_{ion}|f\rangle$, so that

$$V(\mathbf{k}) \approx \langle \mathbf{k}|V_{ion}|f\rangle = \int d^3r e^{-i\mathbf{k}.\mathbf{r}} V_{ion}(r)\psi_f(\mathbf{r}). \tag{15.14}$$

In this way, the only surviving term contributing to the hybridization is the atomic potential - only this term has the high-momentum Fourier components to create a significant overlap between the low momentum conduction electrons and the localized f-state.

Putting these results together, the non-interacting Anderson model can then be written

$$\hat{H}_{resonance} = \sum_\mathbf{k} \overbrace{(E_\mathbf{k} + W - \mu)}^{\epsilon_\mathbf{k}} c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma}(V(\mathbf{k})c^\dagger_{\mathbf{k}\sigma}f_\sigma + \text{H.c}) + \overbrace{(E_f^{ion} - \mu)}^{E_f} n_f.$$

15.3.2 Virtual bound-state formation: the non-interacting resonance.

When the magnetic ion is immersed in a sea of electrons, the f-electrons within the core of the atom can tunnel out, hybridizing with the Bloch states of surrounding electron sea [**?**] as shown in Fig. 15.4.

In the absence of interactions, this physics is described by

$$H_{resonance} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} [V(\mathbf{k}) c^{\dagger}_{\mathbf{k}\sigma} f_{\sigma} + \text{H.c.}] + E_f n_f, \tag{15.15}$$

where $c^{\dagger}_{\mathbf{k}\sigma}$ creates an electron of momentum $\mathbf{k}$, spin σ and energy $\epsilon_{\mathbf{k}} = E_{\mathbf{k}} - \mu$ in the conduction band. The hybridization broadens the localized f-state, and in the absence of interactions, gives rise to a resonance of width Δ given by Fermi's Golden Rule.

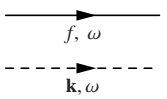
$$\Delta = \pi \sum_{\vec{k}} |V(\mathbf{k})|^2 \delta(\epsilon_{\mathbf{k}} - E_f) \tag{15.16}$$

This is really an average of the density of states $\rho(\epsilon) = \sum_{\mathbf{k}} \delta(\omega - \epsilon_{\mathbf{k}})$ with the hybridization $|V(\mathbf{k})|^2$. For future reference, we shall define

$$\Delta(\epsilon) = \pi \sum_{\vec{k}} |V(\mathbf{k})|^2 \delta(\epsilon_{\mathbf{k}} - \epsilon) = \pi \overline{\rho(\epsilon) V^2(\epsilon)} \tag{15.17}$$

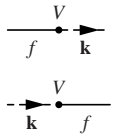
as the "hybridization" function.

Let us now examine the resonant scattering off a non-interacting f-level, using Feynman diagrams. We'll denote the propagator of the bare f-electron by a full line, and that of the conduction electron by a dashed line, as follows:



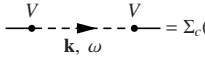
$$G^{(0)}_f(\omega) = \frac{1}{\omega - E_f}$$
$$G^{(0)}(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}}}. \tag{15.18}$$

For simplicity, we will ignore the momentum dependence of the hybridization, taking $V(\mathbf{k}) = V(\mathbf{k})^* \equiv V$. The hybridization is a kind of off-diagonal potential scattering which we denote by a filled dot, as follows:



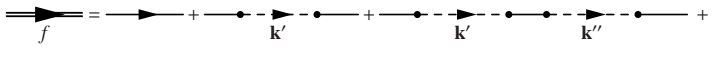
(15.19)

Now the hybridization permits the f-electron to tunnel back and forth into the continuum, a process we can associate with the "self-energy" diagram



$$= \Sigma_c(\omega) = \sum_{\mathbf{k}} \frac{V^2}{\omega - \epsilon_{\mathbf{k}}}. \tag{15.20}$$

We can view this term as an effective scattering potential for the f-electrons, one that is frequency dependent and hence retarded in time, reflecting the fact that an f-electron can spend large amounts of time out in the conduction band. The Feynman diagrams describing the multiple scattering of the f-electron off this potential are then:



(15.21)

Each time the electron tunnels into the conduction band, it does so with a different momentum, so the momenta of the conduction electrons are independently summed over in the intermediate states. As in previous chapters, we can sum these terms as a geometric series to obtain a familiar-looking self-energy correction to the f-propagator.

$$G_f(\omega) = G^{(0)}_f \left[1 + \Sigma_c G^{(0)}_f + \left(\Sigma_c G^{(0)}_f \right)^2 + \ldots \right] = [\omega - E_f - \Sigma_c(\omega)]^{-1} \tag{15.22}$$

Now for a broad conduction band there is a very useful approximation for Σ_c. To derive it, we re-write the momentum sum in the self-energy as an energy integral with the density of states, replacing $\sum_{\mathbf{k}} \to \int d\epsilon \rho(\epsilon)$, so that

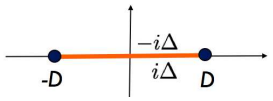
$$\Sigma_c(\omega) = \int \frac{d\epsilon}{\pi} \rho(\epsilon) \frac{\pi V^2}{\omega - \epsilon} = \int \frac{d\epsilon}{\pi} \frac{\Delta(\epsilon)}{\omega - \epsilon}, \tag{15.23}$$

where $\Delta(\epsilon) = \pi \rho(\epsilon) V^2$. In the complex plane, $\Sigma_c(\omega)$ has a branch cut along the real axis with a discontinuity in its imaginary part proportional to the hybridization:

$$Im\Sigma_c(\omega \pm i\delta) = \int \frac{d\epsilon}{\pi} \Delta(\epsilon) \overbrace{\text{Im} \frac{1}{\omega - \epsilon \pm i\delta}}^{\mp i\pi\delta(\omega - \epsilon)}, = \mp \Delta(\omega). \tag{15.24}$$

Consider the particular case where $\Delta(\epsilon) = \Delta$ is constant for $\epsilon \in [-D, D]$, so that

$$\Sigma(\omega \pm i\delta) = \frac{\Delta}{\pi} \int_{-D}^{D} \frac{d\epsilon}{\omega - \epsilon \pm i\delta} = \frac{\Delta}{\pi} \ln \left[\frac{\omega \pm i\delta + D}{\omega \pm i\delta - D} \right]$$



$$= \frac{\Delta}{\pi} \overbrace{\ln \left| \frac{\omega + D}{\omega - D} \right|}^{O(\omega/D)} \mp i\Delta\theta(D - |\omega|) \tag{15.25}$$

which is a function with a branch-cut stretching from $\omega = -D$ to $\omega = +D$. The frequency dependent part of $\text{Re}\Sigma_c = O(\omega/D)$ is negligible in a broad band. We can extend this observation to more general functions $\Delta(\omega)$ that vary slowly over the width of the resonance (lumping any constant part of Σ_c into a shift of E_f.) With this observation, for a broad band, we drop the real part of Σ_c, writing it in the form

$$\Sigma_c(\omega + i\omega') = -i\Delta \text{sgn}(\omega'), \tag{15.26}$$

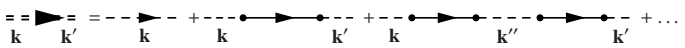
where ω' is the imaginary part of the frequency. (at the Matsubara frequencies, $\Sigma_c(i\omega_n) = -i\Delta \text{sgn}\omega_n$). On the real axis, the f-propagator takes a particularly simple form

$$G_f(\omega - i\delta) = \frac{1}{(\omega - E_f - i\Delta)}, \tag{15.27}$$

that describes a resonance with a width Δ, centered around energy E_f, with a Lorentzian density of states

$$\rho_f(\omega) = \frac{1}{\pi} Im G_f(\omega - i\delta) = \frac{\Delta}{(\omega - E_f)^2 + \Delta^2}.$$

Now let us turn to see how the conduction electrons scatter off this resonance. Consider the repeated scattering of the conduction electrons, represented by the dashed line, off the f-level as follows:



Now using (15.21) we see that third and higher terms can be concisely absorbed into the second term by replacing the bare f-propagator by the full (broadened) f-propagator, as follows

$$G(\mathbf{k}', \mathbf{k}, \omega) = \delta_{\mathbf{k}',\mathbf{k}} G^{(0)}(\mathbf{k}, \omega) + G^{(0)}(\mathbf{k}, \omega) V^2 G_f(\omega) G^{(0)}(\mathbf{k}', \omega) \tag{15.28}$$

We can identify

$$t(\omega) = V^2 G_f(\omega) \tag{15.29}$$

as the scattering t-matrix of the resonance. Infact, this relationship holds quite generally, even when interactions are present, because the only way conduction electrons can scatter, is by passing through the localized f-state. The full conduction electron propagator can then be written

$$G(\mathbf{k}', \mathbf{k}, \omega) = \delta_{\mathbf{k}',\mathbf{k}} G^{(0)}(\mathbf{k}, \omega) + G^{(0)}(\mathbf{k}, \omega) t(\omega) G^{(0)}(\mathbf{k}', \omega). \tag{15.30}$$

Scattering theory tells us that the t-matrix is related to the S-matrix $S(\omega) = e^{2i\delta(\omega)}$, where $\delta(\omega)$ is the scattering phase shift, by the relation $S = 1 - 2\pi i\rho\, t(\omega + i\eta)$(here we use η as the infinitesimal to avoid confusion with the notation for the phase shift), or

$$t(\omega + i\eta) = \frac{1}{-2\pi i\rho}(S(\omega) - 1) = -\frac{1}{\pi\rho} \times \frac{1}{cot\delta(\omega) - i}. \tag{15.31}$$

Substituting our explicit form of the f-Green's function,

$$t(\omega + i\delta) = V^2 G_f(\omega + i\eta) = \frac{1}{\pi\rho} \times \frac{\overbrace{\pi\rho V^2}^{\Delta}}{\omega - E_f + i\Delta} = -\frac{1}{\pi\rho} \times \frac{1}{(\frac{E_f - \omega}{\Delta}) - i} \tag{15.32}$$

Comparing (15.31) and (15.32), we see that scattering phase shift is given by

$$\delta_f(\omega) = \cot^{-1}\left(\frac{E_f - \omega}{\Delta}\right) = \tan^{-1}\left(\frac{\Delta}{E_f - \omega}\right). \tag{15.33}$$

$\delta_f(\omega)$ is a monotonically increasing function, rising from $\delta_f = 0$ at $\omega << 0$ to $\delta_f = \pi$ at high energies. On resonance, $\delta(E_f) = \pi/2$, corresponding to the strongest kind of "unitary scattering".

The Friedel Sum Rule

Remarkably, the phase shift $\delta_f \equiv \delta_f(0)$ at the Fermi surface determines sets the amount of charge bound inside the resonance. Here, we can see this by using the f-spectral function to calculate the ground-state occupancy:

$$n_f = 2\int_{-\infty}^{0} d\omega \rho_f(\omega) = 2\int_{-\infty}^{0} \frac{d\omega}{\pi} \frac{\Delta}{(\omega - E_f)^2 + \Delta^2} = \frac{2}{\pi}\cot^{-1}\left(\frac{E_f}{\Delta}\right) \equiv 2 \times \frac{\delta_f}{\pi}, \tag{15.34}$$

Note that when $\delta(0) = \pi/2$, $n_f = 1$. This is a particular example of the "Friedel sum rule", - a very general relation between the number of particles Δn bound in a potential well and the sum of the scattering phase shifts at the Fermi surface

$$\Delta n = \sum_{\lambda} \frac{\delta_\lambda}{\pi} \tag{15.35}$$

where δ_λ denotes the scattering phase shift in the partial wave state labelled by the orbital quantum numbers λ. [5]

We can understand the Friedel sum rule by looking at the scattering wavefunction far from the impurity. The asymptotic radial wavefunctions of the incoming and the phase-shifted outgoing electrons on the Fermi surface take the form

$$\psi(r) \sim \left[\frac{e^{-ik_F r}}{r} + e^{2i\delta_f}\frac{e^{ik_F r}}{r}\right] \sim \frac{e^{i\delta}\sin(k_F r + \delta_f)}{r}$$

which corresponds to a radial wave in which the wavefunction of the electrons is shifted by an amount

$$\Delta r = -\frac{\delta_f}{k_F} = -\frac{\lambda_F}{2} \times \frac{\delta_f}{\pi}.$$

Thus for a positive phase shift, electrons are *drawn inwards* by the scattering process. Each time δ_f passes through π, one more node of the wavefunction passes through the boundary at infinity, corresponding to an additional bound electron. Anderson has called Friedel's sum rule a "node counting theorem".

[5] For a spherical atom, without spin-orbit coupling $\lambda = (l, m, \sigma)$, where l, m and σ are the angular momentum and spin quantum numbers. With spin orbit coupling, $\lambda = (j, m)$ denote the quantum numbers of total angular momentum j.

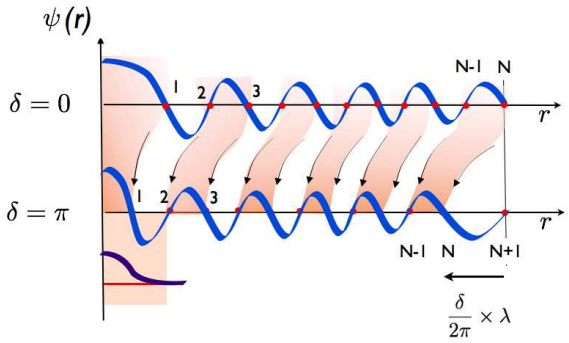


Figure 15.5: Illustrating the Friedel sum rule. As the scattering phase shift grows, the nodes of the eigenstates at the Fermi surface are drawn into the potential well. Each time the phase shift passes through π one more node passes into the well, leading to one more bound-electron.

Example 15.2: Anderson Model as a path integral

Formulate the Anderson model as a path integral and show that the conduction electrons can be "integrated out", giving rise to an action of the following form[**?**]

$$S_F = \sum_{\sigma,i\omega_n} \bar{f}_{\sigma n}\Big\{-i\omega_n + E_f - i\Delta\mathrm{sgn}(\omega_n)\Big\}f_{\sigma n} + \int_0^\beta d\tau U n_\uparrow n_\downarrow. \tag{15.36}$$

where $f_{\sigma n} \equiv \beta^{-\frac{1}{2}}\int_0^\beta d\tau e^{i\omega_n\tau} f_\sigma(\tau)$ is the Fourier transform of the f-electron field.

Solution: We begin by writing the partition function of the Anderson model as a path integral

$$Z = \int \mathcal{D}[f,c]e^{-S} \tag{15.37}$$

where the action $S = S_A + S_B$ is the sum of two terms, an atomic term

$$S_A = \int_0^\beta d\tau[\sum_\sigma \bar{f}_\sigma(\partial_\tau + E_f)f_\sigma + U n_{f\uparrow}n_{f\downarrow}]$$

and a bath term

$$S_B = \int_0^\beta d\tau\left\{\sum_{\mathbf{k}\sigma}\bar{c}_{\mathbf{k}\sigma}(\partial_\tau + \epsilon_{\mathbf{k}\sigma})c_{\mathbf{k}\sigma} + V\left[\bar{f}_\sigma c_{\mathbf{k}\sigma} + \bar{c}_{\mathbf{k}\sigma}f_\sigma\right]\right\} \tag{15.38}$$

describing the hybridization with the surrounding sea of conduction electrons.

We can re-arrange the path integral so that the conduction electron integral is carried out first,

$$Z = \int \mathcal{D}[f]e^{-S_F}\overbrace{\int \mathcal{D}[c]e^{-S_B}}^{Z_B[\{f\}]}, \tag{15.39}$$

where $Z_B[\{f\}]$ contains the change to the f-electron induced by "integrating out" the conduction electrons. The bath action is free of interactions and can be written schematically as a quadratic form

$$S_B = \bar{c}\cdot A\cdot c + \bar{c}\cdot j + \bar{j}\cdot c \tag{15.40}$$

where $A \equiv (\partial_\tau + \epsilon_{\mathbf{k}})\delta(\tau-\tau')$ is the matrix acting on the fields between the fields $c \equiv c_{\mathbf{k}\sigma}(\tau)$ and $\bar{c} = \bar{c}_{\mathbf{k}\sigma}(\tau)$, while $j(\tau) = V f_\sigma(\tau)$ and $\bar{j} = \bar{f}_\sigma(\tau)V$ are source terms. You may find it reassuring to recast S_B in Fourier space, where $A = (-i\omega_n + \epsilon_{\mathbf{k}})$ is explicitly diagonal.

Using the standard result for Gaussian fermion integrals,

$$Z_B = \int \mathcal{D}[c]e^{-\bar{c}Ac - \bar{j}c + \bar{c}j} = \det A \times \exp[\bar{j}.A^{-1}.j].$$

or explicitly,

$$Z_B[\{f\}] = \overbrace{\det[\partial_\tau + \epsilon_{\mathbf{k}}]}^{Z_C = e^{-\beta F_C}}\exp\left[\int_0^\beta d\tau \bar{f}_\sigma\left(\sum_{\mathbf{k}}\frac{V^2}{\partial_\tau + \epsilon_{\mathbf{k}}}\right)f_\sigma\right] \tag{15.41}$$

The first term is the partition function Z_C of the conduction sea in the absence of the magnetic ion. Substituting $Z_B[\{f\}]$ back into the full path integral (15.39) and combining the quadratic terms then gives

$$Z = Z_C \times \int \mathcal{D}[f]\exp\left[-\int d\tau\left\{\bar{f}_\sigma\Big(\partial_\tau + E_f - \sum_{\mathbf{k}}\frac{V^2}{\partial_\tau + \epsilon_{\mathbf{k}}}\Big)f_\sigma + U n_\uparrow n_\downarrow\right\}\right].$$

If we transform the first term into Fourier space, substituting $f_\sigma(\tau) = \beta^{-1/2}\sum_n f_{\sigma n}e^{-i\omega_n\tau}$, $\bar{f}_\sigma(\tau) = \beta^{-1/2}\sum_n \bar{f}_{\sigma n}e^{i\omega_n\tau}$ so that $\partial_\tau \to -i\omega_n$, the action can be written

$$S_F = \sum_{\sigma,i\omega_n}\bar{f}_{\sigma n}\underbrace{\Big\{-i\omega_n + E_f + \overbrace{\sum_{\mathbf{k}}\frac{V^2}{i\omega_n - \epsilon_{\mathbf{k}}}}^{-i\Delta\mathrm{sgn}(\omega_n)}\Big\}}_{-G_f^{-1}(i\omega_n)}f_{\sigma n} + \int_0^\beta d\tau U n_\uparrow n_\downarrow \tag{15.42}$$

The quadratic coefficient of the f-electrons is the inverse f-electron propagator of the non-interacting resonance. We immediately recognize the self-energy term $\Sigma_c(i\omega_n) = -i\Delta\mathrm{sgn}(\omega_n)$ introduced in (15.20). From this path integral derivation, we can see that this term accounts for the effect of the conduction bath electrons, even in the presence of interactions. If we now use the large band-width approximation $\Sigma(i\omega_n) = -i\Delta\mathrm{sgn}\omega_n$ introduced in the (15.26), the action can be compactly written

$$S_F = \sum_{\sigma,i\omega_n}\bar{f}_{\sigma n}\Big\{-i\omega_n + E_f - i\Delta\mathrm{sgn}(\omega_n)\Big\}f_{\sigma n} + \int_0^\beta d\tau U n_\uparrow n_\downarrow. \tag{15.43}$$

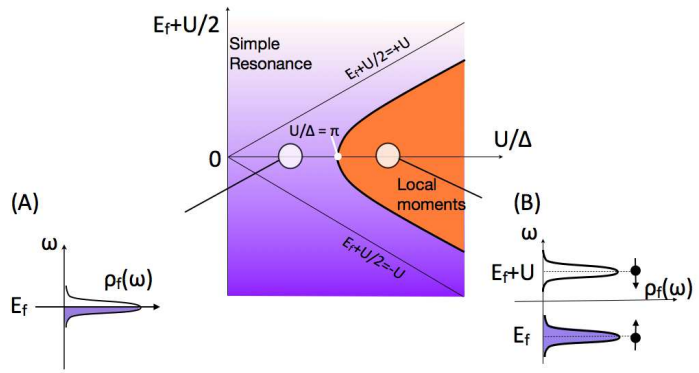


Figure 15.6: Mean field phase diagram of the Anderson model, illustrating how the f-electron resonance splits to form a local moment. A) $U < \pi\Delta$, single half-filled resonance. B) $U > \pi\Delta$, up and down components of the resonance are split by an energy U.

15.3.3 Mean-field theory

In the Anderson model, the Coulomb interaction and hybridization compete with one-another. Crudely speaking, we expect that when the Coulomb interaction exceeds the hybridization, local moments will develop. To gain an initial insight into the effect of hybridization on local moment formation, Anderson originally developed a Hartree mean-field treatment of the repulsive U interaction, decoupling

$$Un_\uparrow n_\downarrow \to Un_\uparrow\langle n_\downarrow\rangle + U\langle n_\uparrow\rangle n_\downarrow - U\langle n_\uparrow\rangle\langle n_\downarrow\rangle + O(\delta n^2). \tag{15.44}$$

We can understand this kind of decoupling procedure as the result of a saddle point description of the path integral, treated in more detail in the following excercise Ex 16.3. Using this mean-field approximation, Anderson concluded that for the symmetric Anderson model, local moments would develop provided

$$U \gtrsim U_c = \pi\Delta. \tag{15.45}$$

Let us now rederive his result. From (15.44), the mean-field effect of the interactions produces a shift the f-level position,

$$E_f \to E_{f\sigma} = E_f + U\langle n_{f-\sigma}\rangle \tag{15.46}$$

which, using (15.34) implies that the scattering phase shift for the up and down channels are no-longer equal, but given by

$$\delta_{f\sigma} = \cot^{-1}\left(\frac{E_{f\sigma}}{\Delta}\right). \tag{15.47}$$

Using the "Friedel sum rule" (15.34), we then obtain the mean-field equations

$$\langle n_{f\sigma}\rangle = \frac{\delta_{f\sigma}}{\pi} = \frac{1}{\pi}\cot^{-1}\left(\frac{E_f + U\langle n_{f-\sigma}\rangle}{\Delta}\right) \tag{15.48}$$

It is convenient to introduce an occupancy $n_f = \sum_\sigma\langle n_{f\sigma}\rangle$ and magnetization $M = \langle n_{f\uparrow}\rangle - \langle n_{f\downarrow}\rangle$, so that $\langle n_{f\sigma}\rangle = \frac{1}{2}(n_f + \sigma M)$ ($\sigma = \pm 1$). The mean-field equation for the occupancy and magnetization are then

$$n_f = \frac{1}{\pi}\sum_{\sigma=\pm1}\cot^{-1}\left(\frac{E_f + U/2(n_f - \sigma M)}{\Delta}\right) \tag{15.49}$$

$$M = \frac{1}{\pi}\sum_{\sigma=\pm1}\sigma\cot^{-1}\left(\frac{E_f + U/2(n_f - \sigma M)}{\Delta}\right) \tag{15.50}$$

To find the critical size of the interaction strength where a local moment develops, we set $M \to 0^+$ in (15.49) to obtain $\frac{E_f + U_c n_f/2}{\Delta} = \cot\left(\frac{\pi n_f}{2}\right)$. Linearing (15.50) in M, we obtain

$$1 = \frac{U_c}{\pi\Delta}\frac{1}{1 + \left(\frac{E_f + Un_f/2}{\Delta}\right)^2} = \frac{U_c}{\pi\Delta}\sin^2\left(\frac{\pi n_f}{2}\right). \tag{15.51}$$

so that for $n_f = 1$,

$$U_c = \pi\Delta \tag{15.52}$$

For larger values of $U > U_c$, there are two solutions, corresponding to an "up" or "down" spin polarization of the f-state. We will see that this is an over-simplified description of the local moment, but it gives us a approximate picture of the physics. The total density of states now contains two Lorentzian peaks, located at $E_f \pm UM$:

$$\rho_f(\omega) = \frac{1}{\pi}\left[\frac{\Delta}{(\omega - E_f - UM)^2 + \Delta^2} + \frac{\Delta}{(\omega - E_f + UM)^2 + \Delta^2}\right]$$

The critical curve obtained by plotting U_c and E_f as a parametric function of n_f is shown in Fig. 15.6.

The Anderson mean-field theory allows a qualitatively understand the experimentally observed formation of local moments. When dilute magnetic ions are dissolved in a metal to form an alloy, the formation of a local moment is dependent on whether the ratio $U/\pi\Delta$ is larger than, or smaller than zero. When iron is dissolved in pure niobium, the failure of the moment to form reflects the higher density of states and larger value of Δ in this alloy. When iron is dissolved in molybdenum, the lower density of states causes $U > U_c$, and local moments form. [**?**]

Example 15.3: Factorizing the interaction in the Anderson model

a) Show that the interaction in the Anderson model can be decoupled via a Hubbard Stratonovich decoupling to yield

$$\int_0^\beta d\tau U n_\uparrow n_\downarrow \to \int_0^\beta d\tau \left[\phi_\uparrow n_\uparrow + \phi_\downarrow n_\downarrow - \frac{\phi_\uparrow \phi_\downarrow}{U}\right] \tag{15.53}$$

where $\phi_\sigma = \phi_0 + i\lambda(\tau) - \sigma h(\tau)$ is the sum of a real and an imaginary field.

b) Derive the mean-field partition function obtained by assuming that the path-integral over ϕ can be approximated by the saddle point configuration where ϕ_σ is independent of time, given by

$$\begin{aligned} Z_{MF} &= \int \mathcal{D}[f] e^{-S_{MF}[\phi_\sigma, f]} \\ S_{MF} &= \sum_{\sigma, i\omega_n} \bar{f}_{\sigma n}[-G^{-1}_{f\sigma}(i\omega_n)] f_{\sigma n} + \frac{\beta}{U}\phi_\uparrow \phi_\downarrow. \end{aligned} \tag{15.54}$$

where

$$G^{-1}_{f\sigma}(i\omega_n) = i\omega_n - E_f - \phi_\sigma + i\Delta \mathrm{sgn}(\omega_n)$$

is the inverse mean-field f-propagator

c) Carry out the Gaussian integral in (15.54) to show that the mean-field free energy is

$$F_{MF} = -k_B T \sum_{\sigma, i\omega_n} \ln\left[-G^{-1}_{f\sigma}(i\omega_n)\right] - \frac{1}{U}\phi_\uparrow \phi_\downarrow.$$

and by setting $\partial F/\partial \phi_\sigma = 0$, derive the mean-field equations

$$\phi_{-\sigma} = U\langle n_{f\sigma}\rangle = U\int_{-\infty}^{\infty} \frac{d\omega}{\pi} f(\omega) \frac{\Delta}{(\omega - E_f - \phi_\sigma)^2 + \Delta^2}.$$

Solution:

a) The interaction in the Anderson model can be rewritten as a sum of two terms,

$$U n_\uparrow n_\downarrow = \overbrace{\frac{U}{4}(n_\uparrow + n_\downarrow)^2}^{\text{“charge”}} - \overbrace{\frac{U}{4}(n_\uparrow - n_\downarrow)^2}^{\text{“spin”}}$$

that we can loosely interpret as a repulsiion between charge fluctuations and an attraction between spin fluctuations. Following the results of Section **.*, inside the path integral, the attractive magnetic interaction can be decoupled in terms of a fluctuating Weiss $h(\tau)$ field, while the the repulsive charge interaction can be decoupled in terms of a fluctuating potential field $\phi(\tau) = \phi_0 + i\lambda(\tau)$, as follows

$$-\frac{1}{2}\times\frac{U}{2}(n_\downarrow - n_\uparrow)^2 \quad\to\quad -h(n_\uparrow - n_\downarrow) + \frac{h^2}{2\times(U/2)},$$

$$+\frac{1}{2}\times\frac{U}{2}(n_\uparrow + n_\downarrow)^2 \quad\to\quad \phi(n_\uparrow + n_\downarrow) - \frac{\phi^2}{2\times(U/2)}, \tag{15.55}$$

with the understanding that for repulsive $U > 0$, fluctuations of $\phi(\tau)$ are integrated along the imaginary axis, $\phi(\tau) = \phi_0 + i\lambda(\tau)$. Adding these terms gives

$$\int_0^\beta d\tau U n_\uparrow n_\downarrow \to \int_0^\beta d\tau \left[(\phi - \sigma h)n_\sigma + \frac{h^2 - \phi^2}{U}\right] = \int_0^\beta d\tau \left[\phi_\uparrow n_\uparrow + \phi_\downarrow n_\downarrow + \frac{\phi_\uparrow \phi_\downarrow}{U}\right] \tag{15.56}$$

where $\phi_\sigma = \phi - \sigma h$. The decoupled path integral then takes the form

$$\begin{aligned} Z_F &= \int \mathcal{D}[\phi_\sigma] \int \mathcal{D}[f] e^{-S_F[\phi_\sigma, f]} \\ S_F &= \int d\tau \left\{ \bar{f}_\sigma \Big(\partial_\tau + E_f + \phi_\sigma - \sum_{\mathbf{k}} \frac{V^2}{\partial_\tau + \epsilon_{\mathbf{k}}}\Big) f_\sigma - \frac{1}{U}\phi_\uparrow \phi_\downarrow \right\}. \end{aligned} \tag{15.57}$$

Note how the Weiss fields ϕ_σ shift the f-level position: $E_f \to E_f + \phi_\sigma(\tau)$. In this way, the Anderson model can be regarded as a resonant level immsersed in a white noise magnetic field that modulates the splitting between the up and down spin resonances.

b) Anderson's mean-field treatment corresponds to to a saddle point approximation to the integral over the ϕ_σ fields. At the saddle point, $\langle \delta S/\delta\phi_\sigma\rangle = 0$. From (15.57), we obtain

$$\frac{\delta S_F}{\delta \phi_\sigma} = \bar{f}_\sigma f_\sigma - \frac{1}{U}\phi_{-\sigma}$$

so the saddle point condition $\langle \delta S_F/\delta\phi_\sigma\rangle = 0$ implies $\phi_{-\sigma} = U\langle n_{f\sigma}\rangle$, recovering the Hartree mean field theory. We can clearly seek solutions in which $\phi_\sigma(\tau) = \phi^{(0)}_\sigma$ is a constant. With this understanding, the saddle point approximation is

$$Z_F \approx Z_{MF} = \int \mathcal{D}[f] e^{-S_F[\phi^{(0)}_\sigma, f]} \tag{15.58}$$

where

$$S_{MF} = \int d\tau \left\{ \bar{f}_\sigma \Big(\partial_\tau + E_f + \phi^{(0)}_\sigma - \sum_{\mathbf{k}} \frac{V^2}{\partial_\tau + \epsilon_{\mathbf{k}}}\Big) f_\sigma - \frac{1}{U}\phi^{(0)}_\uparrow \phi^{(0)}_\downarrow \right\}. \tag{15.59}$$

Now since $\phi^{(0)}$ is a constant, we can Fourier transform the first term in this expression, replacing $\partial_\tau \to -i\omega_n$, to obtain

$$S_{MF} = \sum_{\sigma,\, i\omega_n} \bar{f}_{\sigma n} \overbrace{\Big(-i\omega_n + E_f + \phi^{(0)}_\sigma - \underbrace{\sum_{\mathbf{k}} \frac{V^2}{-i\omega_n + \epsilon_{\mathbf{k}}}}_{-i\mathrm{sgn}(\omega_n)\Delta}\Big)}^{-G^{-1}_{f\sigma}(i\omega_n)} f_{\sigma n} - \frac{\beta}{U}\phi^{(0)}_\uparrow \phi^{(0)}_\downarrow, \tag{15.60}$$

where in the broad-band width limit, we can replace

$$G^{-1}_{f\sigma}(i\omega_n) = i\omega_n - E_f - \phi^{(0)}_\sigma + i\mathrm{sgn}(\omega_n)\Delta. \tag{15.61}$$

c) Carrying out the Gaussian integral in (15.58), we obtain

$$Z_{MF} = \det[-G^{-1}_{f\sigma}(i\omega_n)]e^{\frac{\beta}{U}\phi_\uparrow\phi_\downarrow} = \prod_{\sigma,i\omega_n}[-G^{-1}_{f\sigma}(i\omega_n)]e^{\frac{\beta}{U}\phi_\uparrow\phi_\downarrow},$$

or

$$F_{MF} = -k_BT\ln Z_{MF} = -k_BT\sum_{\sigma,i\omega_n}\ln\left[-G^{-1}_{f\sigma}(i\omega_n)\right]e^{i\omega_n 0^+} - \frac{1}{U}\phi_\uparrow\phi_\downarrow. \qquad (15.62)$$

where we have included the convergence factor $e^{i\omega_n 0^+}$. By (15.61), $\frac{\partial G^{-1}_{f\sigma}(i\omega_n)}{\partial\phi_\sigma} = -1$, so differentiating (15.62) with respect to ϕ_σ, we obtain

$$0 = k_BT\sum_{i\omega_n}G_{f\sigma}(i\omega_n)e^{i\omega_n 0^+} - \frac{1}{U}\phi_{-\sigma}, \qquad (15.63)$$

or

$$\phi_{-\sigma} = U\langle n_{f\sigma}\rangle = Uk_BT\sum_{i\omega_n}G_{f\sigma}(i\omega_n)e^{i\omega_n 0^+}.$$

Carrying out the sum over the Matsubara frequencies by the standard contour integral method, we obtain

$$\begin{aligned}\phi_{-\sigma} &= -U\oint_{\text{Im axis}}\frac{dz}{2\pi i}f(z)G_{f\sigma}(z) = U\oint_{\text{Re axis}}\frac{dz}{2\pi i}f(z)G_{f\sigma}(z)\\ &= U\int_{-\infty}^{\infty}\frac{d\omega}{\pi}f(\omega)\text{Im}G_{f\sigma}(\omega - i\delta)\\ &= U\int_{-\infty}^{\infty}\frac{d\omega}{\pi}f(\omega)\frac{\Delta}{(\omega - E_f - \phi_{0\sigma})^2 + \Delta^2}. \qquad (15.64)\end{aligned}$$

15.3.4 The Coulomb Blockade: local moments in quantum dots

A modern realization of the physics of local moments is found within quantum dots. Quantum dots are a tiny electron pools in a doped semi-conductor, small enough so that the electron states inside the dot are quantized, loosely resembling the electronic states of an atom. Quantum dot behavior also occurs in nanotubes. Unlike a conventional atom, the separation of the electronic states in quantum dot is of the order of milli-electron volts, rather than volts. The overall position of the quantum dot energy levels can be changed by applying a gate voltage to the dot. It is then possible to pass a small current through the dot by placing it between two leads. The differential conductance $G = dI/dV$ is directly proportional to the density of states $\rho(\omega)$ inside the dot $G \propto \rho(0)$. Experimentally, when G is measured as a function of gate voltage V_g, the differential conductance is observed to develop a periodic structure, with a period of a few milli-electron volts. [**?**]

This phenomenon is known as the "Coulomb blockade"[**? ?**] and it results from precisely the same physics that is responsible for moment formation. A simple model for a quantum dot considers it as a sequence of single particle levels at energies ϵ_λ, interacting via a single Coulomb potential U,

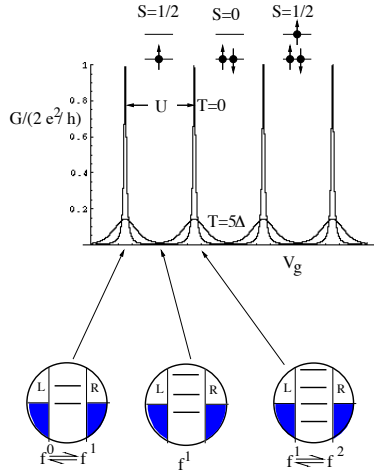


Figure 15.7: Variation of zero bias conductance $G = dI/dV$ with gate voltage in a quantum dot. Coulomb interactions mean that for each additional electron in the dot, the energy to add one electron increases by U. When the charge on the dot is integral, the Coulomb interaction blocks the addition of electrons and the conductance is suppressed. When the energy to add an electron is degenerate with the Fermi energy of the leads, unitary transmission occurs, and for symmetric leads, $G = 2e^2/h$.

according to the model

$$H_{dot} = \sum_\lambda(\epsilon_\lambda + eV_g)n_{\lambda\sigma} + \frac{U}{2}N(N-1) \qquad (15.65)$$

where $n_{\lambda\sigma}$ is the occupancy of the spin σ state of the λ level, $N = \sum_{\lambda\sigma}n_{\lambda\sigma}$ is the total number of electrons in the dot and V_g the gate voltage. This is a simple generalization of the single atom part of the Anderson model. Notice that the capacitance of the dot is $C = e^2/U$.

The energy difference between the n electron and $n+1$ electron state of the dot is given by

$$E(n+1) - E(n) = nU + \epsilon_{\lambda_n} - |e|V_g,$$

where λ_n is the one-particle state into which the n-th electron is being added. As the gate voltage is raised, the quantum dot fills each level sequentially, as illustrated in Fig. 15.7, and when $|e|V_g = nU + \epsilon_{\lambda_n}$, the n-th level becomes degenerate with the Fermi energy of each lead. At this point, electrons can pass coherently through the resonance giving rise to a sharp peak in the conductance. At maximum conductance, the transmission and reflection of electrons is unitary, and the

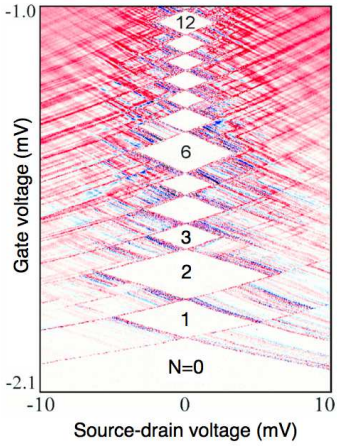


Figure 15.8: Experimentally measured conductance for a voltage-biased quantum dot after [**?**], showing the splitting of the Coulomb blockade into two components, shifted up and down by the voltage bias, $\pm eV_{sd}/2$. In the white diamond-shaped regions, $G(V_{sd}) \approx 0$ as a result of Coulomb blockade. The number of particles N is fixed in each of the diamond regions. The lines outside the diamonds, running parallel to the sides, identify excited states.

conductance of the quantum dot will reach a substantial fraction of the quantum of conductance, e^2/h per spin. A calculation of the zero-temperature conductance through a single non-interacting resonance coupled symmetrically to two leads gives

$$G(V_g) = \frac{2e^2}{h}\frac{\Delta^2}{(\epsilon_\lambda - |e|V_g)^2 + \Delta^2} \tag{15.66}$$

where the factor of two derives from two spin channels. This gives rise to a conductance peak when the gate voltage $|e|V_g = \epsilon_\lambda$. At a finite temperature, the Fermi distribution of the electrons in the leads is thermally broadened, and the conductance involves a thermal average about the Fermi energy

$$G(V_g, T) = \frac{2e^2}{h}\int d\epsilon \left(-\frac{\partial f}{\partial \epsilon}\right)\frac{\Delta^2}{(\epsilon_\lambda - |e|V_g - \epsilon)^2 + \Delta^2} \tag{15.67}$$

where $f(\epsilon) = 1/(e^{\beta\epsilon} + 1)$ is the Fermi function. When there are multiple levels, the each successive

level contributes to the conductance, to give

$$G(V_g, T) = \sum_{n\geq 0}\frac{2e^2}{h}\int d\epsilon \left(-\frac{\partial f}{\partial \epsilon}\right)\frac{\Delta^2}{(nU + \epsilon_{\lambda_n} - |e|V_g - \epsilon)^2 + \Delta^2}$$

where the n-th level is shifted by the Coulomb blockade.

The effect of a bias voltage on these results is interesting. In this situation, the energy distribution function of the two leads are now shifted relative to one-another. An crude model for the effect of a voltage is obtained replacing the Fermi function by an average over both leads, so that $f'(\epsilon) \to \frac{1}{2}\sum_\pm f'(\epsilon \pm \frac{eV_{sd}}{2})$, which has the effect of splitting the conductance peaks into two, peaked at voltages

$$|e|V_g = \epsilon_{\lambda_n} + nU \pm |e|V_{sd}/2 \tag{15.68}$$

as shown in Fig. 15.8.

It is remarkable that the physics of moment formation and the "Coulomb blockade" operate in both artificial mesoscopic devices and naturally occurring magnetic ions.

15.4 The Kondo Effect

Although Anderson's mean-field theory provides a mechanism for moment formation, it raises new questions. While the mean-field treatment of the local moment would be appropriate for an ordered magnet involving a macroscopic number of spins, rigidly locked together, for a single magnetic impurity there will will always be a finite quantum mechanical amplitude for the spin to tunnel between an up and down configuration.

$$e^-_\downarrow + f^1_\uparrow \rightleftharpoons e^-_\uparrow + f^1_\downarrow$$

This tunneling rate τ^{-1}_{sf} defines a temperature scale

$$k_B T_K = \frac{\hbar}{\tau_{sf}}$$

called the Kondo temperature, which sets the cross-over between local moment behavior, where the spin is free, and the low temperature physics, where the spin and conduction electrons are entangled. Historically, the physics of this cross-over posed a major problem for the theoretical physics community that took about a decade to resolve. It turns out that the process by which a local moment disappears or "quenches" at low temperatures is analagous to the physics of quark confinement. Today we name it the "Kondo effect" after the Japanese physicist Jun Kondo who calculated the leading logarithmic contribution that signals this unusual behavior[**?**].

The Kondo effect has a many manifestations in condensed matter physics: not only does it govern the quenching of magnetic moments in a magnetic alloy or a quantum dot[**?**], it is responsible for the formation of heavy fermions in dense Kondo lattice materials (heavy fermion compounds) where the local moments transform into composite quasiparticles with masses sometimes in excess

of a thousand bare electron masses.[**?**] We will see that the Kondo temperature depends exponentially on the strength of the Anderson interaction parameter U. In the symmetric Anderson model, where $E_f = -U/2$,

$$T_K = \sqrt{\frac{2U\Delta}{\pi^2}} \exp\left(-\frac{\pi U}{8\Delta}\right). \tag{15.69}$$

We will derive the key elements of this basic result using perturbative renormalization group reasoning [**?**], but it is also obtained from the exact Bethe ansatz solution of the Anderson model [**? ? ?**].

One can view the physics of local moments from two complimentary perspectives (see Fig. (15.9)):

- an "adiabatic picture" which starts with the non-interacting resonant ground-state ($U = 0$) of the Anderson model, and then considers the effect of dialing up the interaction term U.
- a "scaling approach", which starts with the interacting, but isolated atom ($V(k) = 0$), and considers the effect of immersing it in an electron sea, gradually "integrating out" lower and lower energy electrons.

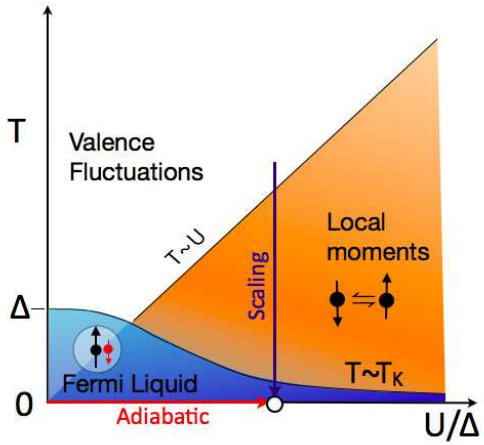


Figure 15.9: The phase diagram of the symmetric Anderson model. Below a scale $T \sim U$ local moments develop. The Kondo temperature T_K plays the role of the renormalized resonant level width. Below a temperature $T \sim T_K$, the local moments become screened by the conduction sea via the Kondo effect, to form a Fermi liquid.

The adiabatic approach involves dialing up the interaction, as shown by the horizontal arrow in figure (15.9). From the adiabatic perspective, the ground-state remains in a Fermi liquid. In principle, one might imagine the possibiity of a phase transition at some finite interaction strength U, but in a single impurity model, with a finite number of local degrees of freedom, we don't expect any symmetry breaking phase transitions. In the scaling approach, we follow the physics as a function of ever-decreasing energy scale, is loosely equivalent to dialing down the temperature, as shown by the vertical arrow in figure (15.9) The scaling approach starts from an atomic perspective:

it allows us to understand the formation of local moments, and at lower temperatures, how a Fermi liquid can develop through the interaction of an isolated magnetic moment with a electron sea.

We shall first discuss one of the most basic manifestations of the Kondo effect: the appearance of a a Kondo resonance in the spectral function of the localized electron. This part of our analysis will involve rather qualitative reasoning based on the ideas of adiabaticity introduced in earlier chapters. Afterwards we adopt the scaling apporach, first deriving derive the Kondo model, describing low-energy coupling between the local moments and conduction electrons by using a "Schrieffer Wolff" transformation of the Anderson model. Finally, we shall discuss the concept of renormalization and apply it to the Kondo model, following the evolution of the physics from the local moment to the Fermi liquid.

15.4.1 Adiabaticity and the Kondo resonance

The adiabatic approach allows us to qualitatively understand the emergence of a remarkable resonance in the excitation spectrum of the localized f-electron - the "Kondo resonance". This resonance is simply the adiabatic renormalization of the Friedel-Anderson resonance seen in the non-interacting Anderson model. Its existence was first infered by Abrikosov and Suhl [**? ?**], but today it is colloquially refered to as the "*Kondo resonance*".

To understand the Kondo resonance we shall study the effects of interactions on the f-spectral function

$$A_f(\omega) = \frac{1}{\pi}\mathrm{Im}G_f(\omega + i\eta) \tag{15.70}$$

where $G_f(\omega - i\delta) =$ is the advanced f-Green's function. From a spectral decomposition (10.7.1) we know that:

$$A_f(\omega) = \begin{cases} \overbrace{\sum_\lambda \left|\langle\lambda|f^\dagger_\sigma|\phi_0\rangle\right|^2 \delta(\omega - [E_\lambda - E_0]),}^{\text{Energy distribution for adding one f-electron.}} & (\omega > 0) \\ \underbrace{\sum_\lambda |\langle\lambda|f_\sigma|\phi_0\rangle|^2\, \delta(\omega - [E_0 - E_\lambda]),}_{\text{Energy distribution for removing f-electron}} & (\omega < 0) \end{cases} \tag{15.71}$$

where E_λ and E_0 are the excited and ground-state energies. For negative energies $\omega < 0$, this spectrum corresponds to the energy spectrum of electrons emitted in X-ray photo-emission, while for positive energies ($\omega > 0$), the spectral function can be measured from inverse X-ray photo-emission [**? ?**]. The weight beneath the Fermi energy determines the f-charge of the ion

$$\langle n_f\rangle = 2\int_{-\infty}^{0} d\omega A_f(\omega) \tag{15.72}$$

In a magnetic ion, such as a Cerium atom in a $4f^1$ state, this quantity is just a little below unity.

Fig. (15.16.) illustrates the effect of the interaction on the f-spectral function. In the non-interacting limit ($U = 0$), the f-spectral function is a Lorentzian of width Δ. If we turn on the interaction U, being careful to shifting the f-level position beneath the Fermi energy to maintain a

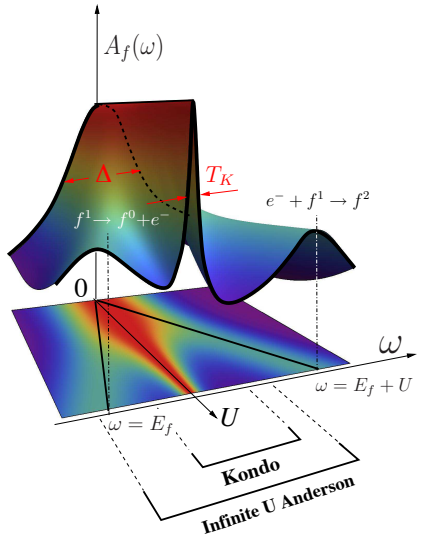


Figure 15.10: Schematic illustrating the formation of a Kondo resonance in the f-spectral function $A_f(\omega)$ as interaction strength U is turned on. Here, the interaction is turned on while maintaining a constant f-occupancy, by shifting the bare f-level position beneath the Fermi energy. The lower part of diagram is the density plot of f-spectral function, showing how the non-interacting resonance at $U = 0$ splits into an upper and lower atomic peak at $\omega = E_f$ and $\omega = E_f + U$.

constant occupancy, the resonance splits into three peaks, two at energies $\omega = E_f$ and $\omega = E_f + U$ corresponding to the energies for a valence fluctuation, plus an additional central "Kondo resonance" associated with the spin-fluctuations of the local moment.

When the interaction is much larger than the hybridization width, $U >> \Delta$, one might expect no spectral weight left at low energies. But it turns out that the spectral function at the Fermi energy is an adiabatic invariant determined by the scattering phase shift δ_f:

$$A_f(\omega = 0) = \frac{\sin^2\delta_f}{\pi\Delta}. \tag{15.73}$$

This result, due to Langreth[**? ?**], guarantees that a "Kondo resonance" is always present at the Fermi energy. Now the total spectral weight $\int_{-\infty}^{\infty} d\omega A_f(\omega) = 1$ is conserved, so if $|E_f|$ and U are both large compared with Δ, most of this weight will be lie far from the Fermi energy, leaving a small residue $Z << 1$ in the Kondo resonance. If the area under the Kondo resonance is Z, since

the height of Kondo resonance is fixed $\sim 1/\Delta$, the renormalized hybridization width Δ^* must be of order $Z\Delta$. This scale is set by the Kondo temperature, so that $Z\Delta \sim T_K$.

The Langreth relation (15.73) follows from the analytic form of the f-Green's function near the Fermi energy. For a single magnetic ion, we expect that the interactions between electrons can be increased continuously, without any risk of instabilities, so that the excitations of the strongly interacting case remain in one-to-one correspondence with the excitations of the non-interacting case $U = 0$, forming a "local Fermi liquid". In this local Fermi liquid, the interactions give rise to an f-electron self-energy, which at zero temperature, takes the form

$$\Sigma_I(\omega - i\eta) = \Sigma_I(0) + (1 - Z^{-1})\omega + iA\omega^2, \tag{15.74}$$

at low energies. As discussed in chapter 8, The quadratic energy dependence of $\Sigma_I(\omega) \sim \omega^2$ follows from the Pauli exclusion principle, which forces a quadratic energy dependence of the phase space for the emission of a particle-hole pair. The "wavefunction" renormalization Z, representing the overlap with the state containing one additional f-quasiparticle, is less than unity, $Z < 1$. Using this result (15.74), the low energy form of the f-electron propagator is

$$\begin{aligned} G_f^{-1}(\omega - i\eta) &= \omega - E_f - i\Delta - \Sigma_I(\omega) = Z^{-1}[\omega - \overbrace{Z(E_f + \Sigma_I(0))}^{E_f^*} - i\overbrace{Z\Delta}^{\Delta^*} - iO(\omega^2)] \\ G_f(\omega - i\eta) &= \frac{Z}{\omega - E_f^* - i\Delta^* - iO(\omega^2)}. \end{aligned} \tag{15.75}$$

This corresponds to a renormalized resonance of reduced weight $Z < 1$, located at postion E_f^* with renormalized width $\Delta^* = Z\Delta$. Now by (15.29) and (15.31), the f-Green's function determines the t-matrix of the conduction electrons $t(\omega + i\eta) = V^2 G_f(\omega + i\eta) = -(\pi\rho)^{-1} e^{i\delta(\omega)} \sin\delta(\omega)$, so the phase of the f-Green's function at the Fermi energy determines the scattering phase shift, δ_f, hence $G_f(0 + i\eta) = (G_f(0 - i\eta))^* = -|G_f(0)|e^{i\delta_f}$. This implies that the scattering phase shift at the Fermi energy is

$$\delta_f = \mathrm{Im}\left(\ln[-G_f^{-1}(\omega - i\eta)]\right)\Big|_{\omega=0} = \tan^{-1}\left\{\frac{\Delta^*}{E_f^*}\right\}. \tag{15.76}$$

Eliminating $E_f^* = \Delta^* \cot\delta_f$ from (15.75), we obtain

$$G_f(0 + i\eta) = -\frac{Z}{\Delta^*} e^{-i\delta_f} \sin\delta_f = -\frac{1}{\Delta} e^{-i\delta_f} \sin\delta_f, \tag{15.77}$$

so that

$$A_f(0) = \frac{1}{\pi}\mathrm{Im}G_f(0 - i\eta) = \frac{\sin^2\delta_f}{\pi\Delta}. \tag{15.78}$$

is an adiabatic invariant.

Photo-emission studies do reveal the three-peaked structure characteristic of the Anderson model in many Ce systems, such as $CeIr_2$ and $CeRu_2$ [**?**] (see Fig. 16.1). Materials in which the Kondo resonance is wide enough to be resolved are more "mixed valent" materials in which the f- valence departs significantly from unity. Three peaked structures have also been observed in certain U 5f

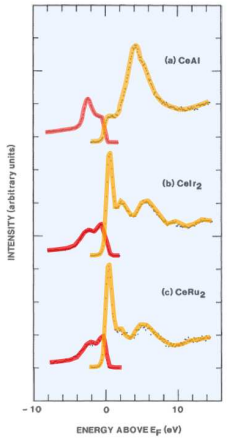


Figure 15.11: Spectral functions for three different Cerium f-electron materials, measured using X-ray photoemission (below the Fermi energy) and inverse X-ray photoemission (above the Fermi energy) after [**?**]. *CeAl* is an antiferromagnet and does not display a Kondo resonance.

materials such as UPt_3 and UAl_2 [**?**]materials, but it has not yet been resolved in UBe_{13}. A three peaked structure has recently been observed in 4f Yb materials, such as $YbPd_3$, where the $4f^{13}$ configuration contains a single f hole, so that the positions of the three peaks are reversed relative to Ce [**?**].

15.4.2 Renormalization concept

The Anderson model illustrates a central theme of condensed matter physics - the existence of physics on several widely spaced energy scales. In particular, the scale at which local moments form is of order the Coulomb energy U, a scale of order $10eV$, while the Kondo effect occurs on a scale a thousand times smaller of order $10K \sim 1meV$. When energy scales are well-separated like this, we use the "renormalization group" to fold the key effects of the high energy physics into a small set of parameters that control the low energy physics. [**? ? ? ?**]

Renormalization is built on the idea that the low energy physics of a system only depend on certain gross features of the high energy physics. The family of systems with the same low energy excitation spectrum constitute a "universality class" of models. (Fig. 15.12) We need the concept of universality, for without without it we would be lost, for we could not hope to capture the physics

of real-world systems with our simplified Hamiltonian models. The Anderson model, is itself a renormalized Hamiltonian, notionally derived from the elimination of high energy excitations from "the" microscopic Hamiltonian.

To carry out renormalization, the Hamiltonian of interest $H(D)$ is parameterized by its cutoff energy scale, D, the energy of the largest excitations. Renormalization involves reducing gthe cutoff to a slightly smaller value $D \to D' = D/b$ where $b > 1$. The excitations in the energy window $E \in [D', D]$ that are removed by this process, are said to have been integrated out of the Hilbert space, and in so doing they give rise to a new "effective" Hamiltonian $\tilde{H}_L$ that continues to faithfully describe the the remaining low-energy degrees of freedom. The energy scales are then rescaled, to obtain a new $H(D') = b\tilde{H}_L$ and the whole process is repeated.

Generically, the Hamiltonian can be divided into a block-diagonal form

$$H = \left[\begin{array}{c|c} H_L & V^\dagger \\ \hline V & H_H \end{array}\right] \tag{15.79}$$

where H_L and H_H act on states in the low-energy and high-energy subspaces respectively, and V and $V^\dagger$ provide the matrix elements between them. The high energy degrees of freedom may be "integrated out" [6] by carrying out a canonical transformation that eliminates the off-diagonal elements in this Hamiltonian $\tilde{H}_L$

$$H(D) \to \tilde{H} = UH(D)U^\dagger = \left[\begin{array}{c|c} \tilde{H}_L & 0 \\ \hline 0 & \tilde{H}_H \end{array}\right] \tag{15.80}$$

One then projects out the low energy component of the block-diagonalized Hamiltonian $\tilde{H}_L = P\tilde{H}P$. Finally, by rescaling

$$H(D') = b\tilde{H}_L \tag{15.81}$$

one arrives at a new Hamiltonian describing the physics on the reduced scale. The transformation from $H(D)$ to $H(D')$ is referred to as a "renormalization group" (RG) transformation. This term was coined long ago, even though the transformation does not form a real group, since there is no inverse transformation.

Repeated application of the RG procedure leads to a family of Hamiltonians $H(D)$. By taking the limit $b \to 1$, these Hamiltonians evolve, or "flow" continuously with D. Typically, H will contain a series of dimensionless parameters (coupling constants) $\{g_i\}$ which denote the strength of various interaction terms in the Hamiltonian. The evolution of these parameters with cut-off is given by a scaling equation. In the the simplest case

$$\frac{\partial g_j}{\partial \ln D} = \beta_j(\{g_i\})$$

A negative β function denotes a "relevant" parameter which grows as the cut-off is reduced. A positive β function denotes an "irrelevant" parameter constant which shrinks towards zero as the cut-off is reduced. There are two types of event that can occur in such a scaling procedure (Fig. 15.14):

[6] The term "integrating out" is originally derived from the path integral formulation of the renormalization group, in which high energy degrees of freedom are removed by integrating over these variables inside the path integral.

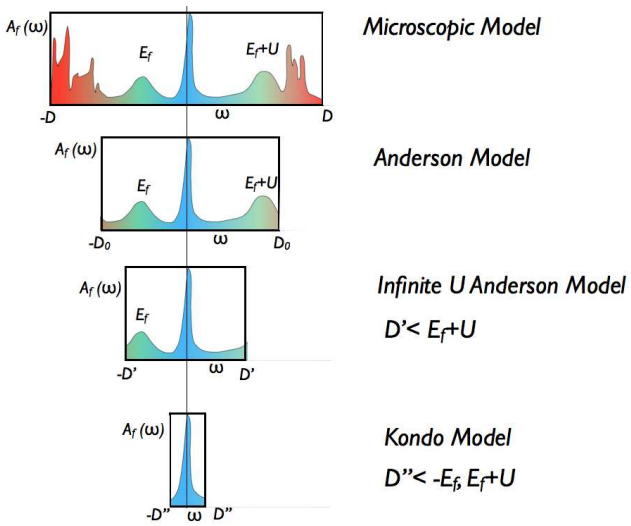


Figure 15.12: Scaling concept. Low energy model Hamiltonians are obtained from the detailed original model by integrating out the high energy degrees of freedom. At each stage, the physics described by the model spans a successively lower frequency window in the excitation spectrum.

- A *crossover*. When the cut-off energy scale D passes the characteristic energy scale of a particular class of high frequency excitations, then at lower energies, these excitations may only occur via a virtual process. When the effects of the virtual fluctuations associated with these high energy process are included into the Hamiltonian, it changes its structure.

- *Fixed Point*. If the cut-off energy scale drops below the lowest energy scale in the problem, then there are no further changes to occur in the Hamiltonian, which will now remain invariant under the scaling procedure (so that the β function of all remaining parameters in the Hamiltonian must vanish). This *"Fixed Point Hamiltonian"* describes the essence of the low energy physics.

Local moment physics involves a sequence of such cross-overs (Fig. 15.12.). The highest energy scales in the Anderson model, are associated with "valence fluctuations" into the empty and doubly occupied states

$$f^1 \;\leftrightharpoons\; f^2 \qquad \Delta E_I = U + E_f > 0$$

$$f^1 \leftrightharpoons f^0 \qquad \Delta E_{II} = -E_f > 0 \tag{15.82}$$

The successive elimination of these processes leads to two cross-overs. Suppose ΔE_I is the largest scale, then once $D < \Delta E_I$, charge fluctuations into the doubly occupied state are eliminated and the remaining low energy Hilbert space of the atom is

$$D < E_f + U: \qquad |f^0\rangle, \qquad |f^1, \sigma\rangle \qquad (\sigma = \pm 1/2) \tag{15.83}$$

The operators that span this space are called "Hubbard operators"[**?**], and they are denoted as follows

$$\begin{aligned} X_{\sigma 0} &= |f^1, \sigma\rangle\langle f^0| = P f^\dagger{}_\sigma, \qquad X_{0\sigma} = |f^0\rangle\langle f^1, \sigma| = f^\dagger{}_\sigma P, \\ X_{\sigma\sigma'} &= |f^1, \sigma\rangle\langle f^1, \sigma'| \end{aligned} \tag{15.84}$$

where $P = (1 - n_{f\uparrow} n_{f\downarrow})$ projects out doubly occupied states. (Note that the Hubbard operators $X_{\sigma 0} = P f^\dagger{}_\sigma$, can not be treated as simple creation operators, for they do not satisfy the canonical anticommutation algebra.) The corresponding renormalized Hamiltonian is the "Infinite U Anderson model",

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + [V(\mathbf{k}) c^\dagger{}_{\mathbf{k}\sigma} X_{0\sigma} + V(\mathbf{k})^* X_{\sigma 0} c_{\mathbf{k}\sigma}] + E_f \sum_\sigma X_{\sigma\sigma}. \tag{15.85}$$

Infinite U Anderson model

In this model, all the interactions are hidden inside the Hubbard operators.

Finally, once $D < \Delta E_{II}$, the low-energy Hilbert space no longer involves the f^2 *or* f^0, states. The object left behind is a quantum top - a quantum mechanical object with purely spin degrees of freedom and a two dimensional[7] Hilbert space

$$|f^1, \sigma\rangle, \qquad (\sigma = \pm 1/2).$$

Now the residual spin degrees of freedom still interact with the surrounding conduction sea, for virtual charge fluctuations, in which an electron temporarily migrates off, or onto the ion lead, to spin-exchange between the local moment and the conduction sea. There are two such virtual processes:

$$\begin{aligned} e_\uparrow + f^1_\downarrow &\leftrightarrow f^2 \leftrightarrow e_\downarrow + f^1_\uparrow \qquad \Delta E_I \sim U + E_f \\ e_\uparrow + f^1_\downarrow &\leftrightarrow e_\uparrow + e_\downarrow \leftrightarrow e_\downarrow + f^1_\uparrow \qquad \Delta E_{II} \sim -E_f \end{aligned} \tag{15.86}$$

[7] In the simplest version of the Anderson model, the local moment is a $S = 1/2$, but in more realistic atoms much large moments can be produced. For example, an electron in a Cerium Ce^{3+} ion atom lives in a $4f^1$ state. Here spin-orbit coupling combines orbital and spin angular momentum into a total angular moment $j = l - 1/2 = 5/2$. The Cerium ion that forms thus has a spin $j = 5/2$ with a spin degeneracy of $2j + 1 = 6$. In multi-electron atoms, the situation can become still more complex, involving Hund's coupling between atoms.

In both cases, spin exchange only takes place in the singlet channel, $S = 0$ state. From second-order perturbation theory, we know that these virtual charge fluctuations will selectively lower the energy of the singlet configurations by an amount of order $\Delta E = -J$, where

$$J \sim V^2 \left[\frac{1}{\Delta E_1} + \frac{1}{\Delta E_2}\right] = V^2 \left[\frac{1}{-E_f} + \frac{1}{E_f + U}\right]. \tag{15.87}$$

Here V is the size of the hybridization matrix element near the Fermi surface. The selective reduction in the energy of the singlet channel constitutes an effective antiferromagnetic interaction between the conduction electrons and the local moment. If we introduce $\vec{\sigma}(0) = \sum_{k,k'} c^\dagger{}_{k\alpha} \vec{\sigma}_{\alpha\beta} c_{k'\beta}$, measuring the the electron spin at the origin, then the effective interaction that lowers the energy of singlet combinations of conduction and f-electrons will have the form $H_{eff} \sim J \vec{\sigma}(0) \cdot \vec{S}_f$. The resulting low-energy Hamiltonian that describes the interaction of a spin with a conduction sea is the deceptively simple "Kondo model"

$$H = \sum_{k\sigma} \epsilon_k c^\dagger{}_{k\sigma} c_{k\sigma} + \overbrace{J \psi^\dagger(0) \vec{\sigma} \psi(0) \cdot \vec{S}_f}^{H_{int}}. \tag{15.88}$$

Kondo model

This heuristic argument was ventured in Anderson's paper on local moment formation in 1961. At the time, the antiferromagnetic sign in this interaction was entirely unexpected, for it had long been that exchange forces always induce a ferromagnetic interaction between the conduction sea and local moments. The innocuous-looking sign difference has deep consequences for the physics of local moments at low temperatures, giving rise to an interaction that grows as the temperature is lowered ultimately leading to a final cross-over into a low-energy Fermi liquid fixed point. The remaining sections of the chapter are devoted to following this process in detail.

15.4.3 Schrieffer-Wolff transformation

We now carry out the transformation that links the Anderson and Kondo models via a canonical transformation, first introduced by Schrieffer and Wolff[**? ?**]. This transformation is a kind of one-step renormalization process in which the valence fluctuations are integrated out of the Anderson model. When a local moment forms, hybridization with the conduction sea induces virtual charge fluctuations. It's useful to consider dividing the Hamiltonian into two terms

$$H = H_1 + \lambda V$$

where λ is an expansion parameter. Here,

$$H_1 = H_{band} + H_{atomic} = \left[\begin{array}{c|c} H_L & 0 \\ \hline 0 & H_H \end{array}\right]$$

is diagonal in the low energy f^1 (H_L) and the high energy f^2 or f^0 (H_H) subspaces, whereas the hybridization term

$$\mathcal{V} = H_{mix} = \sum_{j\sigma}[V_k c^\dagger_{k\sigma} f_\sigma + \text{H.c.}] = \left[\begin{array}{c|c} 0 & V^\dagger \\ \hline V & 0 \end{array}\right]$$

provides the off-diagonal matrix elements between these two subspaces. The idea of the Schrieffer Wolff transformation is to carry out a canonical transformation that returns the Hamiltonian to block-diagonal form:

$$\mathcal{U}\left[\begin{array}{c|c} H_L & \lambda V^\dagger \\ \hline \lambda V & H_H \end{array}\right]\mathcal{U}^\dagger = \left[\begin{array}{c|c} H^* & 0 \\ \hline 0 & H' \end{array}\right]. \tag{15.89}$$

This is a "renormalized" Hamiltonian, and the block-diagonal part of this matrix $H^* = P_L H' P_L$ in the low energy subspace provides an *effective* Hamiltonian for the low energy physics. If we set $\mathcal{U} = e^S$, then $\mathcal{U}^\dagger = \mathcal{U}^{-1} = e^{-S}$ (which implies $S^\dagger = -S$ is anti-hermitian). Writing S as a power series in λ,

$$S = \lambda S_1 + \lambda^2 S_2 + \ldots,$$

then by using the identity, $e^A B e^{-A} = B + [A,B] + \frac{1}{2!}[A,[A,B]]\ldots$, (15.89) can also be expanded in powers of λ as follows

$$e^S(H_1 + \lambda\mathcal{V})e^{-S} = H_1 + \lambda\Big(\mathcal{V} + [S_1, H_1]\Big) + \lambda^2\left(\frac{1}{2}[S_1,[S_1,H]] + [S_1,\mathcal{V}] + [S_2,H_1]\right) + \ldots.$$

Since $\mathcal{V}$ is not diagonal, by requiring

$$[S_1, H_1] = -\mathcal{V}, \tag{15.90}$$

we can eliminate all off-diagonal components to leading order in λ. To second order

$$e^S(H_1 + \lambda\mathcal{V})e^{-S} = H_1 + \lambda^2\left(\frac{1}{2}[S_1,\mathcal{V}] + [S_2,H_1]\right) + \ldots.$$

Since $[S_1,\mathcal{V}]$ is block-diagonal, we can satisfy (15.89) to second order by requiring $S_2 = 0$, so that to this order, the renormalized Hamiltonian has the form

$$H^* = H_L + \lambda^2 H_{int}$$

where

$$H_{int} = \frac{1}{2}P_L[S_1,\mathcal{V}]P_L + \ldots$$

is an interaction term induced by virtual fluctuations into the high-energy manifold. Writing

$$S = \left[\begin{array}{c|c} 0 & -s^\dagger \\ \hline s & 0 \end{array}\right]$$

and substituting into (15.90), we obtain $V = -sH_L + H_H s$. Now since $(H_L)_{ab} = E^L_a\delta_{ab}$ and $(H_H)_{ab} = E^H_a\delta_{ab}$ are diagonal, it follows that

$$s_{ab} = \frac{V_{ab}}{E^H_a - E^L_b}, \qquad -s^\dagger{}_{ab} = \frac{V^\dagger{}_{ab}}{E^L_a - E^H_b}, \qquad . \tag{15.91}$$

From (15.91), we obtain

$$(H_{int})_{ab} = -\frac{1}{2}(V^\dagger s + s^\dagger V)_{ab} = \frac{1}{2}\sum_{\lambda\in|H\rangle}\left[\frac{V^\dagger{}_{a\lambda}V_{\lambda b}}{E^L_a - E^H_\lambda} + \frac{V^\dagger{}_{a\lambda}V_{\lambda b}}{E^L_b - E^H_\lambda}\right]$$

Some important points about this result

- We recognize this result as a simple generalization of second-order perturbation theory to encompass both diagonal and off-diagonal matrix elements.
- H_{int} can also be written

  $$H_{int} = \frac{1}{2}[T(E_a) + T(E_b)]$$

  where T is given by

  $$\begin{aligned} \hat{T}(E) &= P_L\mathcal{V}\frac{P_H}{E - H_1}\mathcal{V}P_L \\ T_{ab}(E) &= \sum_{\lambda\in|H\rangle}\left[\frac{V^\dagger{}_{a\lambda}V_{\lambda b}}{E - E^H_\lambda}\right] \end{aligned} \tag{15.92}$$

  is the leading order expression for the many-body scattering T-matrix induced by scattering off $\mathcal{V}$. We can thus relate H_{int} to a scattering amplitude, and schematically represent it by a Feynman diagram, illustrated in Fig. 15.13.

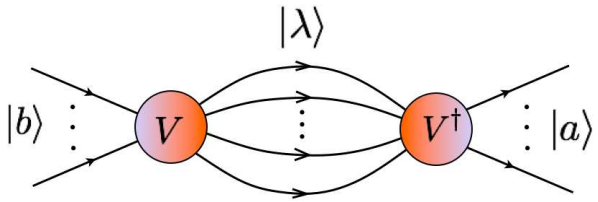


Figure 15.13: T-matrix representation of interaction induced between states $|b\rangle$ and $|a\rangle$ by integrating out the virtual fluctuations into the high-energy states $|\lambda\rangle$.

- If the separation of the low and high energy subspaces is large, then the energy denominators in the above expression will not depend on the initial and final states a and b, so that this expression can be simplified to the form

  $$H_{int} = -\sum_{\lambda\in|H\rangle}\frac{V^\dagger P[\lambda]V}{\Delta E_\lambda} \tag{15.93}$$

where $\Delta E_\lambda = E^H_\lambda - E^L$ is the excitation energy in the high energy subspace labeled by λ, and the projector $P[\lambda] = \sum_{|a\rangle\in|\lambda\rangle} |a\rangle\langle a|$.

We now apply this method to the Anderson model for which the atomic ground-state is a local moment f^1 configuration. In this case, there are two high-energy intermediate states corresponding to f^0 and f^2 configurations. When a conduction electron or hole is excited into the localized f-state to create these excited state configurations, the corresponding excitation energies are $\Delta E(f^1 \to f^0) = -E_f$ and $\Delta E(f^1 \to f^2) = E_f + U$. The hybridization $\mathcal{V} = \sum_{\mathbf{k}\sigma}\left[V(\mathbf{k})c^\dagger_{\mathbf{k}\sigma}f_\sigma + \text{H.c}\right]$ generates virtual fluctuations into these excited states. Using (15.93), the interaction induced by these fluctuations is given by

$$\begin{aligned} H_{int} &= -\frac{VP[f^2]V}{E_f+U} - \frac{VP[f^0]V}{-E_f} \\ &= -\sum_{k\alpha,k'\beta} V^*_{k'}V_k\left[\frac{\overbrace{(c^\dagger_{k\alpha}f_\alpha)(f^\dagger_\beta c_{k'\beta})}^{f^1+e^-\leftrightarrow f^2}}{E_f+U} + \frac{\overbrace{(f^\dagger_\beta c_{k'\beta})(c^\dagger_{k\alpha}f_\alpha)}^{f^1\leftrightarrow f^0+e^-}}{-E_f}\right]P_{n_f=1} \end{aligned} \tag{15.94}$$

where $P_{n_f=1} = (n_{f\uparrow} - n_{f\downarrow})^2$ projects into the subspace of unit occupancy. Using the Fierz identity[8] $2\delta_{\alpha\gamma}\delta_{\eta\beta} = \delta_{\alpha\beta}\delta_{\eta\gamma} + \vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\eta\gamma}$ we may recast the spin exchange terms in terms of Pauli matrices as follows

$$\begin{aligned} (c^\dagger_{k\alpha}f_\alpha)(f^\dagger_\beta c_{k'\beta}) &= (c^\dagger_{k\alpha}f_\gamma)(f^\dagger_\eta c_{k'\beta})\times \overbrace{(\delta_{\alpha\gamma}\delta_{\eta\beta})}^{\frac{1}{2}(\delta_{\alpha\beta}\delta_{\eta\gamma}+\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\eta\gamma})} \\ &= \frac{1}{2}c^\dagger_{k\alpha}c_{k'\alpha} - (c_{k\alpha}{}^\dagger\vec{\sigma}_{\alpha\beta}c_{k'\beta})\cdot\vec{S}_f, \end{aligned} \tag{15.95}$$

and similarly

$$(f^\dagger_\beta c_{k'\beta})(c^\dagger_{k\alpha}f_\alpha) = -\frac{1}{2}c^\dagger_{k\alpha}c_{k'\alpha} - (c_{k\alpha}{}^\dagger\vec{\sigma}_{\alpha\beta}c_{k'\beta})\cdot\vec{S}_f. \tag{15.96}$$

(where we have replaced $n_f = 1$ and dropped residual constants in both cases). The operator

$$\vec{S}_f \equiv f^\dagger_\sigma\left(\frac{\vec{\sigma}_{\alpha\beta}}{2}\right)f_\beta, \qquad (n_f = 1) \tag{15.97}$$

describes the spin of the f-electron. The renormalized Hamiltonian then becomes

$$\begin{aligned} H_{int} &= \sum_{k\alpha,k'\beta} J_{k,k'}c^\dagger_{k\alpha}\vec{\sigma}c_{k'\beta}\cdot\vec{S}_f + H' \\ J_{k,k'} &= V^*_{k'}V_k\left[\overbrace{\frac{1}{E_f+U}}^{f^1+e^-\leftrightarrow f^2} + \overbrace{\frac{1}{-E_f}}^{f^1\leftrightarrow f^0+e^-}\right]. \end{aligned} \tag{15.98}$$

[8] This identity is obtained by expanding an arbitrary two dimensional matrix A in terms of Pauli matrices. If we write $A_{\alpha\beta} = \frac{1}{2}\text{Tr}[A\underline{1}]\delta_{\alpha\beta} + \frac{1}{2}\text{Tr}[A\vec{\sigma}]\cdot\vec{\sigma}_{\alpha\beta}$ and read off the coefficients of A inside the traces, we obtain the inequality.

Notice how, in the low energy subspace, the occupancy of the f-state is constrained to $n_f = 1$. This fermionic representation (15.97) of the spin operator proves to be very useful. Apart from a constant, the second term

$$H' = -\frac{1}{2}\sum_{k,k'\sigma} V^*_{k'}V_k\left[\frac{1}{E_f+U} + \frac{1}{E_f}\right]c^\dagger_{k\sigma}c_{k'\sigma}$$

is a residual potential scattering term off the local moment. This term vanishes for the particle-hole symmetric case $E_f = -(E_f+U)$ and will be dropped, since it does not involve the internal dynamics of the local moment. Summarizing, the effect of the high-frequency valence fluctuations is to induce an antiferromagnetic coupling between the local spin density of the conduction electrons and the local moment:

$$H = \sum_{k\sigma}\epsilon_k c^\dagger_{k\sigma}c_{k\sigma} + \sum_{k,k'}J_{k,k'}c^\dagger_{k\alpha}\vec{\sigma}c_{k'\beta}\cdot\vec{S}_f \tag{15.99}$$

This is the famous "Kondo model". For many purposes, the k dependence of the coupling constant can be dropped, so that the Kondo model takes the deceptively simple form

$$H = \sum_{k\sigma}\epsilon_k c^\dagger_{k\sigma}c_{k\sigma} + \overbrace{J\vec{\sigma}(0)\cdot\vec{S}_f}^{H_{int}}. \tag{15.100}$$

Kondo model

where $\psi_\alpha(0)\sum c_{k\alpha}$ is the electron operator at the origin and $\psi^\dagger(0)\vec{\sigma}\psi(0)$ is the spin density at the origin. In other words, there is a simple point-interaction between the spin density of the metal at the origin and the local moment.

15.4.4 "Poor Man" Scaling

We now apply the scaling concept to the Kondo model. This was originally carried out by Anderson and Yuval[**? ? ?**] using a method formulated in the time, rather than energy domain. The method presented here follows Anderson's " Poor Man's" scaling approach[**? ?**], in which the evolution of the coupling constant is followed as the band-width of the conduction sea is reduced. The Kondo model is written

$$\begin{aligned} H &= \sum_{|\epsilon_k|<D}\epsilon_k c^\dagger_{k\sigma}c_{k\sigma} + H^{(I)} \\ H^{(I)} &= J(D)\sum_{|\epsilon_k|,|\epsilon_{k'}|<D} c^\dagger_{k\alpha}\vec{\sigma}_{\alpha\beta}c_{k'\beta}\cdot\vec{S}_f \end{aligned} \tag{15.101}$$

where the density of conduction electron states $\rho(\epsilon)$ is taken to be constant. The Poor Man's renormalization procedure follows the evolution of $J(D)$ that results from reducing D by progressively integrating out the electron states at the edge of the conduction band. In the Poor Man's procedure, the band-width is not rescaled to its original size after each renormalization, which avoids the need to renormalize the electron operators so that instead of Eq. (15.81), $H(D') = \bar{H}_L$.

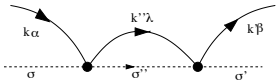
To carry out the renormalization procedure, we integrate out the high-energy spin fluctuations using the t-matrix formulation for the induced interaction H_{int}, derived in the last section. Formally, the induced interaction is given by

$$\delta H^{int}_{ab} = \frac{1}{2}[T_{ab}(E_a) + T_{ab}(E_b)]$$

where

$$T_{ab}(E) = \sum_{\lambda\in|H\rangle}\left[\frac{H^{(I)}_{a\lambda}H^{(I)}_{\lambda b}}{E - E^H_\lambda}\right]$$

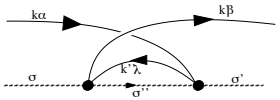
where the energy of state $|\lambda\rangle$ lies in the range $[D', D]$. There are two possible intermediate states that can be produced by the action of $H^{(I)}$ on a one-electron state: (I) either the electron state is scattered directly, or (II) a virtual electron hole-pair is created in the intermediate state. In process (I), the T-matrix can be represented by the Feynman diagram



for which the T-matrix for scattering into a high energy electron state is

$$\begin{aligned} T^{(I)}(E)_{k'\beta\sigma';k\alpha\sigma} &= \sum_{\epsilon_{k''}\in[D-\delta D,D]}\left[\frac{1}{E-\epsilon_{k''}}\right]J^2(\sigma^a\sigma^b)_{\beta\alpha}(S^aS^b)_{\sigma'\sigma} \\ &\approx J^2\rho\delta D\left[\frac{1}{E-D}\right](\sigma^a\sigma^b)_{\beta\alpha}(S^aS^b)_{\sigma'\sigma} \end{aligned} \qquad (15.102)$$

In process (II),



the formation of a particle-hole pair involves a conduction electron line that crosses itself, leading to a negative sign. Notice how the spin operators of the conduction sea and antiferromagnet reverse their relative order in process II, so that the T-matrix for scattering into a high-energy hole-state is given by

$$T^{(II)}(E)_{k'\beta\sigma';k\alpha\sigma} = -\sum_{\epsilon_{k''}\in[-D,-D+\delta D]}\left[\frac{1}{E-(\epsilon_k+\epsilon_{k'}-\epsilon_{k''})}\right]J^2(\sigma^b\sigma^a)_{\beta\alpha}(S^aS^b)_{\sigma'\sigma}$$

$$= -J^2\rho\delta D\left[\frac{1}{E-D}\right](\sigma^b\sigma^a)_{\beta\alpha}(S^aS^b)_{\sigma'\sigma} \qquad (15.103)$$

where we have assumed that the energies ϵ_k and $\epsilon_{k'}$ are negligible compared with D. Adding (Eq. 15.102) and (Eq. 15.103) gives

$$\begin{aligned} \delta H^{int}_{k'\beta\sigma';k\alpha\sigma} &= \hat{T}^I + \hat{T}^{II} = -\frac{J^2\rho\delta D}{D}[\sigma^a,\sigma^b]_{\beta\alpha}S^aS^b \\ &= \frac{J^2\rho\delta D}{D}\vec{\sigma}_{\beta\alpha}\vec{S}_{\sigma'\sigma}. \end{aligned} \qquad (15.104)$$

In this way we see that the virtual emission of a high energy electron and hole generates an antiferromagnetic correction to the original Kondo coupling constant

$$J(D') = J(D) + 2J^2\rho\frac{\delta D}{D}$$

High frequency spin fluctuations thus *antiscreen* the antiferrromagnetic interaction. If we introduce the coupling constant $g = \rho J$, we see that it satisfies

$$\frac{\partial g}{\partial \ln D} = \beta(g) = -2g^2 + O(g^3).$$

This is an example of a negative β function: a signature of an interaction which is weak at high frequencies, but which grows as the energy scale is reduced. The local moment coupled to the conduction sea is said to be asymptotically free. The solution to this scaling equation is

$$g(D') = \frac{g_o}{1 - 2g_o\ln(D/D')} \qquad (15.105)$$

and if we introduce the scale

$$T_K = D\exp\left[-\frac{1}{2g_o}\right] \qquad (15.106)$$

we see that this can be written

$$2g(D') = \frac{1}{\ln(D'/T_K)}$$

This is an example of a running coupling constant- a coupling constant whose strength depends on the scale at which it is measured. (See Fig. 15.14).

Were we to take this equation literally, we would say that g diverges at the scale $D' = T_K$. This interpretation is too literal, because the above scaling equation has only been calculated to order g^2, nevertheless, this result does show us that the Kondo interaction can only be treated perturbatively at energy scales large compared with the Kondo temperature. We also see that once we have written the coupling constant in terms of the Kondo temperature, all reference to the original cut-off energy scale vanishes from the expression. This cut-off independence of the problem is an indication that the physics of the Kondo problem does not depend on the high energy details of the model: there is only one relevant energy scale, the Kondo temperature.

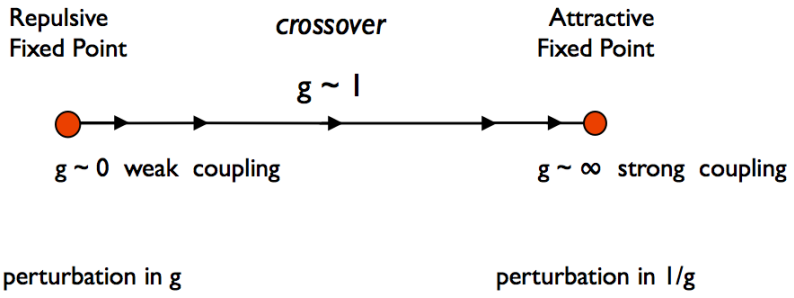


Figure 15.14: Schematic illustration of renormalization group flow from a repulsive "weak coupling" fixed point, via a crossover to an attractive "strong coupling" fixed point.

It is possible to extend the above leading order renormalization calculation to higher order in g. To do this requires a more systematic method of calculating higher order scattering effects. One tool that is particularly useful in this respect, is to use the Abrikosov pseudo-fermion representation of the spin, writing

$$\begin{aligned} \vec{S} &= f^\dagger_\alpha \left(\frac{\vec{\sigma}}{2}\right)_{\alpha\beta} f_\beta \\ n_f &= 1. \end{aligned} \tag{15.107}$$

This has the advantage that the spin operator, which does not satisfy Wick's theorem, is now factorized in terms of conventional fermions. Unfortunately, the second constraint is required to enforce the condition that $S^2 = 3/4$. This constraint proves very awkward for the development of a Feynman diagram approach. One way around this problem, is to use the Popov trick, whereby the f-electron is associated with a complex chemical potential

$$\mu = -i\pi\frac{T}{2}$$

The partition function of the Hamiltonian is written as an unconstrained trace over the conduction and pseudofermion Fock spaces,

$$Z = \mathrm{Tr}\left[e^{-\beta(H+i\pi\frac{T}{2}(n_f-1))}\right] \tag{15.108}$$

Now since the Hamiltonian conserves n_f, we can divide this trace up into contributions from the d^0, d^1 and d^2 subspaces, as follows:

$$Z = e^{i\pi/2}Z(f^0) + Z(f^1) + e^{-i\pi/2}Z(f^2)$$

But since $S_f = 0$ in the $f^2$and d^0 subspaces, $Z(f^0) = Z(f^2)$ so that the contributions to the partition function from these two unwanted subspaces exactly cancel. You can test this method by applying it to a free spin in a magnetic field. (see exercise)

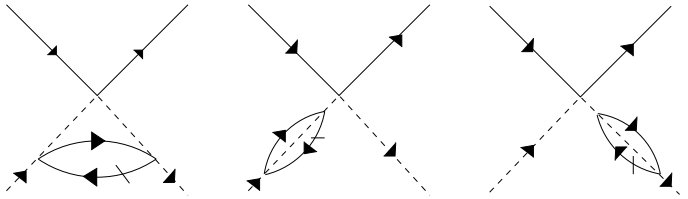


Figure 15.15: Diagrams contributing to the third-order term in the beta function. A "crossed" propagator line indicates that the contribution from high-energy electrons with energies $|\epsilon_k| \in [D - \delta D, D]$ is taken from this line.

By calculating the higher order diagrams shown in fig 15.15 , it is straightforward, though laborious to show that the beta-function to order g^3 is given by

$$\frac{\partial g}{\partial \ln D} = \beta(g) = -2g^2 + 2g^3 + O(g^4) \tag{15.109}$$

One can integrate this equation to obtain

$$\ln\left(\frac{D'}{D}\right) = \int_{g_o}^{g}\frac{dg'}{\beta(g')} = -\frac{1}{2}\int_{g_o}^{g} dg\left[\frac{1}{g'^2} + \frac{1}{g'} + O(1)\right]$$

A better estimate of the temperature T_K where the system scales to strong coupling is obtained by setting $D' = T_K$ and $g = 1$ in this equation, which gives

$$\ln\left(\frac{T_K}{\tilde{D}}\right) = -\frac{1}{2g_o} + \frac{1}{2}\ln 2g_o + O(1), \tag{15.110}$$

where for convenience, we have absorbed a factor $\sqrt{\frac{e}{2}}$ into the cut-off, writing $\tilde{D} = D\sqrt{\frac{e}{2}}$. Thus,

$$T_K = \tilde{D}\sqrt{2g_o}e^{-\frac{1}{2g_o}} \tag{15.111}$$

up to a constant factor. The square-root pre-factor in T_K is often dropped in qualitative discussion, but it is important for more quantitative comparison.

15.4.5 Universality and the resistance minimum

Provided the Kondo temperature is far smaller than the cut-off, then at low energies it is the only scale governing the physics of the Kondo effect. For this reason, we expect all physical quantities

to be expressed in terms of universal functions involving the ratio of the temperature or field to the Kondo scale. For example, the susceptibility

$$\chi(T) = \frac{1}{4T}F(\frac{T}{T_K}), \tag{15.112}$$

and the quasiparticle scattering rate

$$\frac{1}{\tau(T)} = \frac{1}{\tau_o}\mathcal{G}(\frac{T}{T_K}) \tag{15.113}$$

both display universal behavior.

We can confirm the existence of universality by examining these properties in the weak coupling limit, where $T >> T_K$. Here, we find

$$\begin{aligned}\frac{1}{\tau(T)} &= 2\pi J^2\rho S(S+1)n_i, \qquad (S=\frac{1}{2})\\ \chi(T) &= \frac{n_i}{4T}\left[1-2J\rho\right]\end{aligned}$$

where n_i is the density of impurities. Scaling implies that at lower temperatures $J\rho \to J\rho + 2(J\rho)^2\ln\frac{D}{T}$, so that to next leading order we expect

$$\frac{1}{\tau(T)} = n_i\frac{2\pi}{\rho}S(S+1)[J\rho + 2(J\rho)^2\ln\frac{D}{T}]^2, \tag{15.114}$$

$$\chi(T) = \frac{n_i}{4T}\left[1-2J\rho-4(J\rho)^2\ln\frac{D}{T}+O((J\rho)^3)\right] \tag{15.115}$$

results that are confirmed from second-order perturbation theory. The first result was obtained by Jun Kondo. Kondo was looking for a consequence of the antiferromagnetic interaction predicted by the Anderson model, so he computed the electron scattering rate to third order in the magnetic coupling. The logarithm which appears in the electron scattering rate means that as the temperature is lowered, the rate at which electrons scatter off magnetic impurities rises. It is this phenomenon that gives rise to the famous Kondo "resistance minimum" .

Since we know the form of T_K, we can use this result to deduce that the weak coupling limit of the scaling forms. If we take equation (15.110), and replace the cut-off by the temperature $D \to T$, and replace g_o by the running coupling constant $g_o \to g(T)$, we obtain

$$g(T) = \frac{1}{2\ln\left(\frac{T}{T_K}\right) + \ln 2g(T)} \tag{15.116}$$

which we may iterate to obtain

$$2g(T) = \frac{1}{\ln\left(\frac{T}{T_K}\right)} + \frac{\ln(\ln(T/T_K))}{2\ln^2\left(\frac{T}{T_K}\right)}. \tag{15.117}$$

Using this expression to make the replacement $J\rho \to g(T)$ in (15.114) and (15.115), we obtain

$$\chi(T) = \frac{n_i}{4T}\left[1-\frac{1}{\ln(T/T_K)}-\frac{1}{2}\frac{\ln(\ln(T/T_K))}{\ln^2(T/T_K)}+\dots\right] \tag{15.118}$$

$$\frac{1}{\tau(T)} = n_i\frac{\pi S(S+1)}{2\rho}\left[\frac{1}{\ln^2(T/T_K)}+\frac{\ln(\ln(T/T_K))}{\ln^3(T/T_K)}+\dots\right] \tag{15.119}$$

From the second result, we see that the electron scattering rate has the scale-invariant form

$$\frac{1}{\tau(T)} = \frac{n_i}{\rho}\mathcal{G}(T/T_K). \tag{15.120}$$

where $\mathcal{G}(x)$ is a universal function. The pre-factor in the electron scattering rate is essentially the Fermi energy of the electron gas: it is the "unitary scattering" rate, the maximum possible scattering rate that is obtained when an electron experiences a resonant $\pi/2$ scattering phase shift. From this result, we see that at absolute zero, the electron scattering rate will rise to the value $\frac{1}{\tau}(T) = \frac{n_i}{\rho}\mathcal{G}(0)$, indicating that at strong coupling, the scattering rate is of the same order as the unitary scattering limit. We shall now see how this same result comes naturally out of a strong coupling analysis.

15.4.6 Nozières Fermi Liquid Theory of the Kondo Ground-state

The weak-coupling analysis tells us that at scales of order the Kondo temperature, the Kondo coupling constant g scales to a value of order $O(1)$. Although perturbative renormalization group methods can not go past this point, Anderson and Yuval[**? ? ?**]pointed out that it is not unreasonable to suppose that the Kondo coupling constant scales to a fixed point where it is large compared to the conduction electron band-width D. This assumption is the simplest possibility and if true, it means that the strong-coupling limit is an attractive fixed point, being stable under the renormalization group. Anderson and Yuval conjectured that the Kondo singlet would be paramagnetic, with a temperature independent magnetic susceptibility and a universal linear specific heat given by $C_V = \gamma_K\frac{T}{T_K}$ at low temperatures.

The first controlled treatment of this cross-over regime was carried out by Wilson using a numerical renormalization group method. Wilson's numerical renormalization method was able to confirm the conjectured renormalization of the Kondo coupling constant to infinity. This limit is called the "strong coupling" limit of the Kondo problem. Wilson carried out an analysis of the strong-coupling limit, and was able to show that the specific heat would be a linear function of temperature, like a Fermi liquid. Wilson showed that the linear specific heat could be written in a universal form

$$\begin{aligned}C_V &= \gamma T,\\ \gamma &= \frac{\pi^2}{3}\frac{0.4128\pm 0.002}{8T_K}\end{aligned} \tag{15.121}$$

Wilson also compared the ratio between the magnetic susceptibility and the linear specific heat with the corresponding value in a non-interacting system, computing

$$W = \frac{\chi/\chi^0}{\gamma/\gamma^0} = \frac{\chi}{\gamma}\left(\frac{\pi^2k_B^2}{3(\mu_B)^2}\right) = 2 \tag{15.122}$$

within the accuracy of the numerical calculation.

Remarkably, the second result of Wilson's can be re-derived using an exceptionally elegant set of arguments due to Nozières[**?**] that leads to an explicit form for the strong coupling fixed point

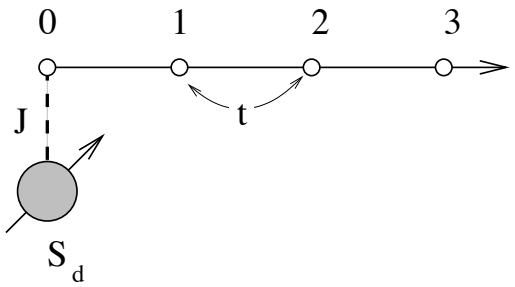


Figure 15.16: Illustrating the strong-coupling limit of the Kondo model

Hamiltonian. Nozières began by considering an electron in a one-dimensional chain as illustrated in Fig. 15.16. The Hamiltonian for this situation is

$$H_{lattice} = -t \sum_{j=0,\infty} [c^\dagger{}_\sigma(j+1)c_\sigma(j) + \text{H.c}] + Jc^\dagger{}_\alpha(0)\vec{\sigma}_{\alpha\beta}c_\beta(0)\cdot\vec{S_f}. \tag{15.123}$$

Nozières argued that the strong coupling fixed point will be described by the situation $J >> t$. In this limit, the kinetic energy of the electrons in the band can be treated as a perturbation to the Kondo singlet. The local moment couples to an electron at the origin, forming a "Kondo singlet" denoted by

$$|GS\rangle = \frac{1}{\sqrt{2}}(|\Uparrow\downarrow\rangle - |\Downarrow\uparrow\rangle) \tag{15.124}$$

where the thick arrow refers to the spin state of the local moment and the thin arrow refers to the spin state of the electron at site 0. Any electron which migrates from site 1 to site 0 will automatically break this singlet state, raising its energy by $3J/4$. This will have the effect of excluding electrons (or holes) from the origin. The fixed point Hamiltonian must then take the form

$$H_{lattice} = -t \sum_{j=1,\infty} [c^\dagger{}_\sigma(j+1)c_\sigma(j) + \text{H.c}] + \text{weak interaction} \tag{15.125}$$

where the second-term refers to the weak-interactions induced in the conduction sea by virtual fluctuations onto site 0. If the wavefunction of electrons far from the impurity has the form $\psi(x) \sim \sin(k_F x)$, where k_F is the Fermi momentum, then the exclusion of electrons from site 1 has the effect of phase-shifting the electron wavefunctions by one the lattice spacing a, so that now $\psi(x) \sim \sin(k_F x - \delta)$ where $\delta = k_F a$. But if there is one electron per site, then $2(2k_F a/(2\pi)) = 1$ by the Luttinger sum rule, so that $k_F = \pi/(2a)$ and hence the Kondo singlet acts as a spinless, elastic scattering center with scattering phase shift

$$\delta = \pi/2. \tag{15.126}$$

The appearance of $\delta = \pi/2$ could also be deduced by appealing to the Friedel sum rule, which states that the number of bound-electrons at the magnetic impurity site is $\sum_\sigma \frac{\delta_{\sigma=\pm1}}{\pi} = 2\delta/\pi$, so that $\delta = \pi/2$. By considering virtual fluctuations of electrons between site 1 and 0, Nozières argued that the induced interaction at site 1 must take the form

$$H_{int} \sim \frac{t^4}{J^3} n_{1\uparrow} n_{1\downarrow} \tag{15.127}$$

because fourth order hopping processes lower the energy of the singly occupied state, but they do not occur for the doubly occupied state. This is a repulsive interaction amongst the conduction electrons, and it is known to be a marginal operator under the renormalization group, leading to the conclusion that the effective Hamiltonian describes a weakly interacting "local" Fermi liquid.

Nozières formulated this local Fermi liquid in the language of an occupancy-dependent phase shift. Suppose the $k\sigma$ scattering state has occupancy $n_{k\sigma}$, then the the ground-state energy will be a functional of these occupancies $E[\{n_{k\sigma}\}]$. The differential of this quantity with respect to occupancies defines a *phase shift* as follows

$$\frac{\delta E}{\delta n_{k\sigma}} = \epsilon_k - \frac{\Delta\epsilon}{\pi}\delta(\{n_{k'\sigma'}\}, \epsilon_k). \tag{15.128}$$

The first term is just the energy of an unscattered conduction electron, while $\delta(\{n_{k'\sigma'}\}, \epsilon_k)$ is the scattering phase shift of the Fermi liquid. This phase shift can be expanded

$$\delta(\{n_{k'\sigma'}\}, \epsilon_k) = \frac{\pi}{2} + \alpha(\epsilon_k - \mu) + \Phi\sum_k \delta n_{k,-\sigma} \tag{15.129}$$

where the term with coefficient Φ describes the interaction between opposite spin states of the Fermi liquid. Nozières argued that when the chemical potential of the conduction sea is changed, the occupancy of the localized d state will not change, which implies that the phase shift is invariant under changes in μ. Now under a shift $\delta\mu$, the change in the occupancy $\sum_k \delta n_{k\sigma} \to \delta\mu\rho$, so that changing the chemical potential modifies the phase shift by an amount

$$\Delta\delta = (\alpha + \Phi\rho)\Delta\mu = 0 \tag{15.130}$$

so that $\alpha = -\rho\Phi$. We are now in a position to calculate the impurity contribution to the magnetic susceptibility and specific heat. First note that the density of quasiparticle states is given by

$$\rho = \frac{dN}{dE} = \rho_o + \frac{1}{\pi}\frac{\partial\delta}{\partial\epsilon} = \rho_o + \frac{\alpha}{\pi} \tag{15.131}$$

so that the low temperature specific heat is given by $C_V = (\gamma_{bulk} + \gamma_i)$ where

$$\gamma_i = 2\left(\frac{\pi^2 k_B^2}{3}\right)\frac{\alpha}{\pi} \tag{15.132}$$

where the prefactor "2" is derived from the spin up and spin-down bands. Now in a magnetic field, the impurity magnetization is given by

$$M = \frac{\delta_\uparrow}{\pi} - \frac{\delta_\downarrow}{\pi} \tag{15.133}$$

Since the Fermi energies of the up and down quasiparticles are shifted to $\epsilon_{F\sigma} \to \epsilon_F - \sigma B$, we have $\sum_k \delta n_{k\sigma} = \sigma\rho B$, so that the phase-shift at the Fermi surface in the up and down scattering channels becomes

$$\begin{aligned}\delta_\sigma &= \frac{\pi}{2} + \alpha\delta\epsilon_{F\sigma} + \Phi(\sum_k \delta n_{k\sigma} \\ &= \frac{\pi}{2} + \alpha\sigma B - \Phi\rho\sigma B \\ &= \frac{\pi}{2} + 2\alpha\sigma B \end{aligned} \tag{15.134}$$

so that the presence of the interaction term doubles the size of the change in the phase shift due to a magnetic field. The impurity magnetization then becomes

$$M_i = \chi_i B = 2\left(\frac{2\alpha}{\pi}\right)\mu_B^2 B \tag{15.135}$$

where we have reinstated the magnetic moment of the electron. This is twice the value expected for a "rigid" resonance, and it means that the Wilson ratio is

$$W = \frac{\chi_i \pi^2 k_B^2}{\gamma_i 3(\mu_B)^2} = 2 \tag{15.136}$$

15.4.7 Experimental observation of Kondo effect

Experimentally, there is now a wealth of observations that confirm our understanding of the single impurity Kondo effect. Here is a brief itemization of some of the most important observations. (Fig. 15.17.)

- A resistance minimum appears when local moments develop in a material. For example, in $Nb_{1-x}Mo_x$ alloys, a local moment develops for $x > 0.4$, and the resistance is seen to develop a minimum beyond this point.[**?** **?**]
- Universality seen in the specific heat $C_V = \frac{n_i}{T}F(T/T_K)$ of metals doped with dilute concentrations of impurities. Thus the specific heat of $\underline{Cu} - Fe$ (iron impurities in copper) can be superimposed on the specific heat of $\underline{Cu} - Cr$, with a suitable rescaling of the temperature scale. [**?** **?**]
- Universality is observed in the differential conductance of quantum dots[**?** **?**] and spin-fluctuation resistivity of metals with a dilute concentration of impurities.[**?**] Actually, both properties are dependent on the same thermal average of the imaginary part of the scattering T-matrix

$$\begin{aligned}\rho_i &= n_i \frac{ne^2}{m}\int d\omega \left(-\frac{\partial f}{\partial \omega}\right) 2Im[T(\omega)] \\ G &= \frac{2e^2}{\hbar}\int d\omega \left(-\frac{\partial f}{\partial \omega}\right)\pi\rho Im[T(\omega)].\end{aligned} \tag{15.137}$$

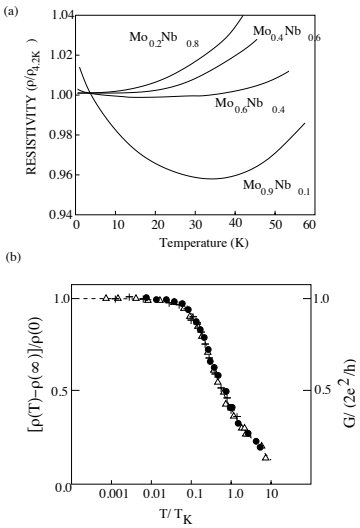


Figure 15.17: (a) Sketch of resistance minimum in Mo_xNb_{1-x} (b) Sketch of excess resistivity associated with scattering from an impurity spin. Right hand-scale- differential conductivity of a quantum dot.

Putting $\pi\rho\int d\omega\left(-\frac{\partial f}{\partial\omega}\right)\mathrm{Im}T(\omega) = t(\omega/T_K, T/T_K)$, we see that both properties have the form

$$\begin{aligned}\rho_i &= n_i\frac{2ne^2}{\pi m\rho}t(T/T_K) \\ G &= \frac{2e^2}{\hbar}t(T/T_K)\end{aligned} \tag{15.138}$$

where $t(T/T_K)$ is a universal function. This result is born out by experiment.

15.5 Exercises

1. (a) Using the identity $n_{f\sigma}^2 = n_{f\sigma}$, show that the atomic part of the Anderson model can be written in the form

$$H_{atomic} = (E_f + \frac{U}{2})n_f + \frac{U}{2}\Big[(n_f - 1)^2 - 1\Big], \tag{15.139}$$

What happens when $E_f + U/2 = 0$?

(b) Using the completeness relation

$$\overbrace{|f^0\rangle\langle f^0|+|f^2\rangle\langle f^2|}^{} \quad \overbrace{|\uparrow\rangle\langle\uparrow|+|\downarrow\rangle\langle\downarrow|}^{}$$
$$(n_f-1)^2 \quad + \frac{\mathbf{S}^2}{S(S+1)} = 1. \qquad (S=1/2)$$

show that the interaction can also be written in the form

$$H_{atomic} = (E_f + \frac{U}{2})n_f - \frac{2U}{3}\mathbf{S}^2 \tag{15.140}$$

which makes it clear that the repulsive U term induces a "magnetic attraction" that favors formation of a local moment.

(c) Derive the Hubbard Stratonovich decoupling for (16.54).

2. By expanding a plane wave state in terms of spherical harmonics:

$$\langle \mathbf{r}|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi\sum_{l,m} i^l j_l(kr)Y^*_{lm}(\hat{\mathbf{k}})Y_{lm}(\hat{\mathbf{r}})$$

show that the overlap between a state $|\psi\rangle$ with wavefunction $\langle \vec{x}|\psi\rangle = R(r)Y_{lm}(\hat{r})$ with a plane wave is given by $V(\vec{k}) = \langle\vec{k}|V|\psi\rangle = V(k)Y_{lm}(\hat{k})$ where

$$V(k) = 4\pi i^{-l}\int dr r^2 V(r)R(r)\, j_l(kr) \tag{15.141}$$

3. (i) Show that $\delta = \cot^{-1}\left(\frac{E_d}{\Delta}\right)$ is the scattering phase shift for scattering off a resonant level at position E_d.

(ii) Show that the energy of states in the continuum is shifted by an amount $-\Delta\epsilon\delta(\epsilon)/\pi$, where $\Delta\epsilon$ is the separation of states in the continuum.

(iii) Show that the increase in density of states is given by $\partial\delta/\partial E = \rho_d(E)$. (See chapter 3.)

4. Generalize the scaling equations to the anisotropic Kondo model with an anisotropic interaction

$$H_I = \sum_{|\epsilon_k|,|\epsilon_{k'}|,a=(x,y,z)} J^a c^\dagger_{k\alpha}\sigma^a_{\alpha\beta}c_{k'\beta}\cdot S^a{}_d \tag{15.142}$$

and show that the scaling equations take the form

$$\frac{\partial J_a}{\partial \ln D} = -2J_bJ_c\rho + O(J^3),$$

where and (a,b,c) are a cyclic permutation of (x,y,z). Show that in the special case where $J_x = J_y = J_\perp$, the scaling equations become

$$\begin{aligned}\frac{\partial J_\perp}{\partial \ln D} &= -2J_zJ_\perp\rho + O(J^3),\\ \frac{\partial J_z}{\partial \ln D} &= -2(J_z)^2\rho + O(J^3),\end{aligned} \tag{15.143}$$

so that $J_z^2 - J_\perp^2$ = constant. Draw the corresponding scaling diagram.

5. Consider the symmetric Anderson model, with a symmetric band-structure at half filling. In this model, the d^0 and d^2 states are degenerate and there is the possibility of a "charged Kondo effect" when the interaction U is negative. Show that under the "particle-hole" transformation

$$\begin{aligned} c_{k\uparrow} &\rightarrow c_{k\uparrow}, \qquad d_\uparrow \rightarrow d_\uparrow\\ c_{k\downarrow} &\rightarrow -c^\dagger{}_{k\downarrow}, \qquad d_\downarrow \rightarrow -d^\dagger{}_\downarrow\end{aligned} \tag{15.144}$$

the positive U model is transformed to the negative U model. Show that the spin operators of the local moment are transformed into Nambu "isospin operators" which describe the charge and pair degrees of freedom of the d-state. Use this transformation to argue that when U is negative, a charged Kondo effect will occur at exactly half-filling involving quantum fluctuations between the degenerate d^0 and d^2 configurations.

6. What happens to the Schrieffer-Wolff transformation in the infinite U limit? Rederive the Schrieffer-Wolff transformation for an N-fold degenerate version of the infinite U Anderson model. This is actually valid for Ce and Yb ions.

7. Rederive the Nozières Fermi liquid picture for an SU (N) degenerate Kondo model. Explain why this picture is relevant for magnetic rare earth ions such as Ce^{3+} or Yb^{3+}.

8. Check the Popov trick works for a magnetic moment in an external field. Derive the partition function for a spin in a magnetic field using this method.

9. Use the Popov trick to calculate the T-matrix diagrams for the leading Kondo renormalization diagramatically.

10. Derive the formula (15.66) for the conductance of a single isolated resonance.

11. (a) Directly confirm the Read-Newn's gauge transformation (16.41).

(b) Directly calculate the "phase stiffness" $\rho_\phi = -\frac{d^2F}{d\lambda^2}$ of the large N Kondo model and show that at $T = 0$.

$$\rho_\phi = \frac{N}{\pi}\left(\frac{\sin(\pi q)}{T_K}\right).$$

12. (a) Introduce a simple relaxation time into the conduction electron propagator, writing

$$G(\vec{k}, i\omega_n)^{-1} = i\omega_n + i\mathrm{sgn}(\omega_n)/2\tau + \frac{V^2}{i\omega_n - \lambda} \tag{15.145}$$

Show that the poles of this Greens function occur at

$$\omega = E_k \pm \frac{i}{2\tau^*}$$

where

$$\tau^* = \frac{m^*}{m}\tau$$

is the renormalized elestic scattering time.

(b) The Kubo formula for the optical conductivity of an isotropic one-band system is

$$\sigma(\nu) = -\frac{Ne^2}{3}\sum_k v_k^2 \frac{\Pi(\nu)}{i\nu}$$

where we have used the N fold spin degeneracy, and $\Pi(\nu)$ is the analytic extension of

$$\Pi(i\nu_n) = T\sum_m G(\vec{k}, i\omega_m)\Big[G(\vec{k}, i\omega_m + i\nu_n) - G(\vec{k}, i\omega_m)\Big]$$

where in our case, $G(\vec{k}, i\omega_n)$ is the conduction electron propagator. Using (16.59), and approximating the momentum sum by an integral over energy, show that the low frequency conductivity of the large N Kondo lattice is given by

$$\sigma(\nu) = \frac{ne^2}{m^*}\frac{1}{(\tau^*)^{-1} - i\nu}.$$

Chapter 16

Heavy electrons

16.1 Doniach's Kondo lattice hypothesis

Although the single impurity Kondo problem was essentially solved by the early seventies, it took a further decade before the physics community was ready to accept the notion that the same phenomenon could occur within a dense lattice environment. This resistance to change was rooted in a number of popular misconceptions about the spin physics and the Kondo effect.

At the beginning of the seventies, it was well known that local magnetic moments severely suppress superconductivity, so that typically, a few percent is all that is required to destroy the superconductivity. Conventional superconductivity is largely immune to the effects of non-magnetic disorder [1] but highly sensitive to magnetic impurities, which destroy the time-reversal symmetry necessary for s-wave pairing. The arrival of a new class of superconducting material containing dense arrays of local moments took the physics community completely by surprise. Indeed, the first observations of superconductivity in UBe_{13}, made in 1973 [1] were dismissed as an artifact and had to await a further ten years before they were revisited and acclaimed as heavy fermion superconductivity. [2, 3]

Normally, local moment systems develop antiferromagnetic order at low temperatures. When a magnetic moment is introduced into a metal it induces Friedel oscillations in the spin density around the magnetic ion, given by

$$\langle \vec{M}(x)\rangle = -J\chi(\vec{x}-\vec{x}')\langle \vec{S}(\vec{x}')\rangle$$

where J is the strength of the Kondo coupling and

$$\chi(x) \;=\; \sum_{\vec{q}} \chi(\vec{q}) e^{i\vec{q}\cdot\vec{x}}$$

[1] Anderson argued in his "dirty superconductor theorem" that BCS superconductivity involves pairing of electrons in states that are the time-reverse transform of one another. Non-magnetic disorder does not break time reversal symmetry, and so the one particle eigenstates of a dirty system can still be grouped into time-reverse pairs from which s-wave pairs can be constructed. For this reason, s-wave pairing is largely unaffected by non-magnetic disorder.

$$\chi(\vec{q}) \;=\; 2\sum_{\vec{k}} \frac{f(\epsilon_{\vec{k}}) - f(\epsilon_{\vec{k}+\vec{q}})}{\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}} \tag{16.1}$$

is the the non-local susceptibility of the metal. If a second local moment is introduced at location

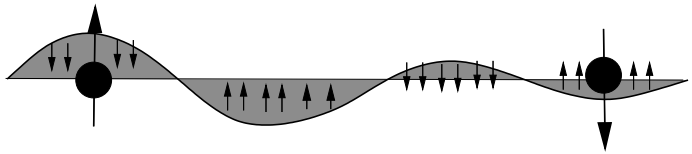


Figure 16.1: Illustrating how the polarization of spin around a magnetic impurity gives rise to Friedel oscillations and induces an RKKY interaction between the spins

$\vec{x}$, then it couples to $\langle M(\vec{x})\rangle$ giving rise to a long-range magnetic interaction called the "RKKY"[4] interaction, [2]

$$H_{RKKY} = \overbrace{-J^2\chi(\vec{x}-\vec{x}')}^{J_{RKKY}(\vec{x}-\vec{x}')}\vec{S}(x)\cdot\vec{S}(x'). \tag{16.2}$$

The sharp discontinuity in the occupancies at the Fermi surface produces slowly decaying Friedel oscillations in the RKKY interaction given by

$$J_{RKKY}(r) \sim -J^2\rho\frac{\cos 2k_F r}{|k_F r|^3} \tag{16.3}$$

where ρ is the conduction electron density of states and r is the distance from the impurity, so the RKKY interaction oscillates in sign, depending on the distance between impurities. The approximate size of the RKKY interaction is given by $E_{RKKY} \sim J^2\rho$.

Normally, the oscillatory nature of this magnetic interaction favors the development of antiferromagnetism. In alloys containing a dilute concentration of magnetic transition metal ions, the RKKY interaction gives rise to a frustrated, glassy magnetic state known as a spin glass in which the magnetic moments freeze into a fixed, but random orientation. In dense systems, the RKKY interaction typically gives rise to an ordered antiferromagnetic state with a Néel temperature $T_N \sim J^2\rho$.

In 1976 Andres, Ott and Graebner discovered the heavy fermion metal $CeAl_3$. [**?**] This metal has the following features:

- A Curie susceptibility $\chi^{-1} \sim T$ at high temperatures.
- A paramagnetic spin susceptibility $\chi \sim constant$ at low temperatures.
- A linear specific heat capacity $C_V = \gamma T$, where $\gamma \sim 1600 mJ/mol/K^2$ is approximately 1600 times larger than in a conventional metal.

[2] named after Ruderman, Kittel, Kasuya and Yosida

- A quadratic temperature dependence of the low temperature resistivity $\rho = \rho_o + AT^2$

Andres, Ott and Grabner pointed out that the low temperature properties are those of a Fermi liquid, but one in which the effective masses of the quasiparticles are approximately 1000 larger than the bare electron mass. The Fermi liquid expressions for the magnetic susceptibility χ and the linear specific heat coefficient γ are

$$\begin{aligned} \chi &= (\mu_B)^2 \frac{N^*(0)}{1+F_o^a} \\ \gamma &= \frac{\pi^2 k_B^2}{3} N^*(0) \end{aligned} \tag{16.4}$$

where $N^*(0) = \frac{m^*}{m} N(0)$ is the renormalized density of states and F_0^a is the spin-dependent part of the s-wave interaction between quasiparticles. What could be the origin of this huge mass renormalization? Like other Cerium heavy fermion materials, the Cerium atoms in this metal are in a $Ce^{3+}(4f^1)$ configuration, and because they are spin-orbit coupled, they form huge local moments with a spin of $J = 5/2$. In their paper, Andres, Ott and Graebner suggested that a lattice version of the Kondo effect might be responsible.

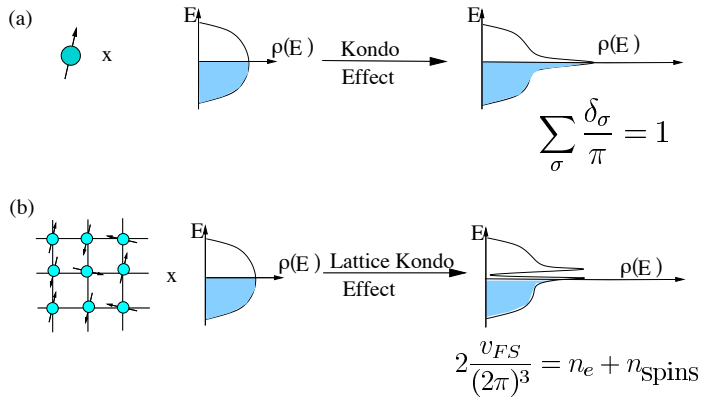


Figure 16.2: (a) Single impurity Kondo effect builds a single fermionic level into the conduction sea, which gives rise to a resonance in the conduction electron density of states (b) Lattice Kondo effect builds a fermionic resonance into the conduction sea in each unit cell. The elastic scattering off this lattice of resonances leads to formation of a heavy electron band, of width T_K.

This discovery prompted Sebastian Doniach[**?**] to propose that the origin of these heavy electrons derived from a dense version of the Kondo effect. Doniach proposed that heavy electron

systems should be modeled by the "Kondo-lattice Hamiltonian" where a dense array of local moments interact with the conduction sea. For a Kondo lattice with spin 1/2 local moments, the Kondo lattice Hamiltonian[**?**] takes the form

$$H = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + J \sum_j \vec{S}_j \cdot c^\dagger_{\vec{k}\alpha} \left(\frac{\vec{\sigma}}{2}\right)_{\alpha\beta} c_{\vec{k}'\beta} e^{i(\vec{k}'-\vec{k})\cdot\vec{R}_j} \tag{16.5}$$

Doniach argued that there are two scales in the Kondo lattice, the Kondo temperature T_K and E_{RKKY}, given by

$$\begin{aligned} T_K &= De^{-1/2J\rho} \\ E_{RKKY} &= J^2\rho \end{aligned} \tag{16.6}$$

When $J\rho$ is small, then $E_{RKKY} >> T_K$, and an antiferromagnetic state is formed, but when the

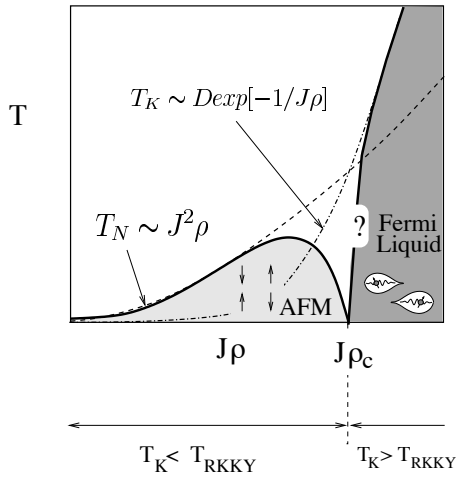


Figure 16.3: Doniach diagram, illustrating the antiferromagnetic regime, where $T_K < T_{RKKY}$ and the heavy fermion regime, where $T_K > T_{RKKY}$. Experiment has told us in recent times that the transition between these two regimes is a quantum critical point. The effective Fermi temperature of the heavy Fermi liquid is indicated as a solid line. Circumstantial experimental evidence suggests that this scale drops to zero at the antiferromagnetic quantum critical point, but this is still a matter of controversy.

Kondo temperature is larger than the RKKY interaction scale, $T_K >> E_{RKKY}$, Doniach argued that a

dense Kondo lattice ground-state is formed in which each site resonantly scatters electrons. Bloch's theorem then insures that the resonant elastic scattering at each site will form a highly renormalized band, of width $\sim T_K$. By contrast to the single impurity Kondo effect, in the heavy electron phase of the Kondo lattice the strong elastic scattering at each site acts in a coherent fashion, and does not give rise to a resistance. For this reason, as the heavy electron state forms, the resistance of the system drops towards zero. One of the fascinating aspects of the Kondo lattice concerns the

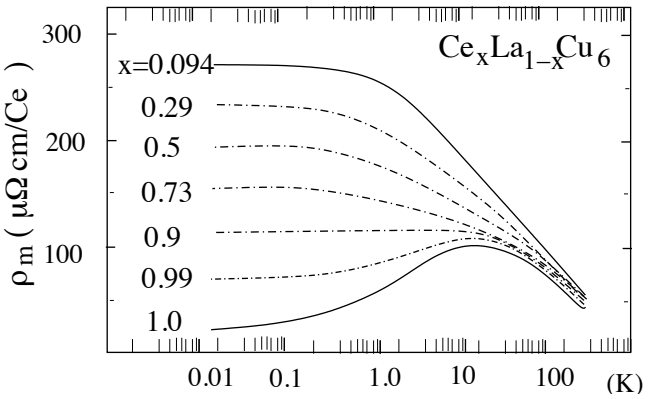


Figure 16.4: Development of coherence in heavy fermion systems. Resistance in $Ce_{1-x}La_xCu_6$ after Onuki and Komatsubara[**?**]

Luttinger sum rule. This aspect was first discussed in detail by Martin[5], who pointed out that the Kondo model can be regarded as the result of adiabatically increasing the interaction strength U in the Anderson model, whilst preserving the valence of the magnetic ion. During this process, one expects sum rules to be preserved. In the impurity, the scattering phase shift at the Fermi energy counts the number of localized electrons, according to the Friedel sum rule

$$\sum_\sigma \frac{\delta_\sigma}{\pi} = n_f = 1$$

This sum rule survives to large U, and reappears as the constraint on the scattering phase shift created by the Abrikosov Suhl resonance. In the lattice, the corresponding sum rule is the Luttinger sum rule, which states that the Fermi surface volume counts the number of electrons, which at small U is just the number of localized (4f, 5f or 3d) and conduction electrons. When U becomes large, number of localized electrons is now the number of spins, so that

$$2\frac{\mathcal{V}_{FS}}{(2\pi)^3} = n_e + n_{\rm spins}$$

This sum rule is thought to hold for the Kondo lattice Hamiltonian, independently of the origin of the localized moments. Such a sum rule would work, for example, even if the spins in the model were derived from nuclear spins, provided the Kondo temperature were large enough to guarantee a paramagnetic state.

Experimentally, there is a great deal of support for the above picture. It is possible, for example, to examine the effect of progressively increasing the concentration of Ce in the non-magnetic host $LaCu_6$.(16.4) At dilute concentrations, the resistivity rises to a maximum at low temperatures. At dense concentrations, the resistivity shows the same high temperature behavior, but at low temperatures coherence between the sites leads to a dramatic drop in the resistivity. The thermodynamics of the dense and dilute system are essentially identical, but the transport properties display the effects of coherence.

There are many indications that the Fermi surface of heavy electron systems has a volume which counts both spins and conduction electrons. The most direct evidence derives from Fermi surface studies made from accurate measurements of de Haas van Alphen oscillations [**? ?**]. Typically, in the heavy Fermi liquid, the measured de Haas van Alphen orbits are consistent with band-structure calculations in which the f-electrons are assumed to be delocalized. By contrast, the measured masses of the heavy electrons often exceed the band-structure calculated masses of the narrow f-band by an order of magnitude or more. Perhaps the most remarkable discovery of recent years, is the observation that the volume of the f-electron Fermi surface appears to "jump" to a much smaller value when the f-electrons anti-ferro magnetically order, indicating that once the Kondo effect is interupted by magnetism, the heavy f-electrons become localized again[**?**]

Yet Doniach scenario for heavy fermion development is fundamentally a comparison of energy scales: it does not tell us how the heavy fermion phase evolves from the antiferromagnet, nor does it explain the nature of the heavy f-electron. Amongst the early objections to Doniach's hypothesis and were of particular concern:

- Size of the Kondo temperature T_K. Simple estimates of the value of $J\rho$ required for heavy electron behavior give a value $J\rho \sim 1$. Yet in the Anderson model, $J\rho \sim 1$ would imply a mixed valent situation, with no local moment formation.

- Exhaustion paradox. The naive picture of the Kondo model imagines that the local moment is screened by conduction electrons within an energy range T_K of the Fermi energy. The number of conduction electrons in this range is of order $T_K/D << 1$ per unit cell, where D is the band-width of the conduction electrons, suggesting that there are not enough conduction electrons to screen the local moments.

The resolution of these two issues are quite intriguing.

Enhancement of the Kondo temperature by spin degeneracy

The resolution of the first issue has its origins in the large spin-orbit coupling of the rare earth or actinide ions in heavy electron systems. This protects the orbital angular momentum against quenching by the crystal fields. Rare earth and actinide ions consequently display a large total

angular momentum degeneracy $N = 2j + 1$, which has the effect of dramatically enhancing the Kondo temperature. Take for example the case of the Cerium ion, where the $4f^1$ electron is spin-orbit coupled into a state with $j = 5/2$, giving a spin degeneracy of $N = 2j+1 = 6$. Ytterbium heavy fermion materials involve the $Yb : 4f^{13}$ configuration, which has an angular momentum $j = 7/2$, or $N = 8$.

To take account of these large spin degeneracies, we need to generalize the Kondo model. This was done in the mid-sixties by Coqblin and Schrieffer[6]. Coqblin and Schrieffer considered a degenerate version of the infinite U Anderson model in which the spin component of the electrons runs from $-j$ to j,

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + E_f \sum_\sigma |f^1:\sigma\rangle\langle f^1:\sigma| + \sum_{k,\sigma} V\left[c^\dagger_{k\sigma}|f^0\rangle\langle f^1:\sigma| + \text{H.c.}\right].$$

Here the conduction electron states are also labeled by spin indices that run from $-j$ to j. This is because the spin-orbit coupled f states couple to partial wave states of the conduction electrons in which the orbital and spin angular momentum are combined into a state of definite j. Suppose $|\vec{k}\sigma\rangle$ represents a plane wave of momentum $\vec{k}$, then one can construct a state of definite orbital angular momentum l by integrating the plane wave with a spherical harmonic, as follows:

$$|klm\sigma\rangle = \int \frac{d\Omega}{4\pi} |\vec{k}\sigma\rangle Y^*_{lm}(\hat{k})$$

When spin orbit interactions are strong, one must work with a partial wave of definite j, obtained by combining these states in the following linear combinations. Thus for the case $j = l + 1/2$ (relevant for Ytterbium ions), we have

$$|km\rangle = \sum_{\sigma=\pm1} \sqrt{\frac{l+\sigma m+\frac{1}{2}}{2l+1}} |klm - \frac{\sigma}{2}, \frac{\sigma}{2}\rangle.$$

An electron creation operator is constructed in a similar way. This construction is unfortunately, not simultaneously possible at more than one site.

When $E_f << 0$, the valence of the ion approaches unity and $n_f \to 1$. In this limit, one can integrate out the virtual fluctuations $f^1 \rightleftharpoons f^0 + e^-$ via a Schrieffer Wolff transformation. This leads to the Coqblin Schrieffer model

$$H_{CS} = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J \sum_{k,k',\alpha\beta} c^\dagger_{k\beta} c_{k'\alpha} \Gamma_{\alpha\beta}, \qquad (\sigma,\alpha,\beta \in [-j, j]).$$

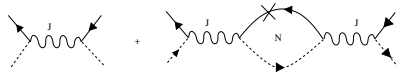
where $J = V^2/|E_f|$ is the induced antiferromagnetic interaction strength. This interaction is understood as the result of virtual charge fluctuations into the f^0 state, $f^1 \rightleftharpoons f^0 + e^-$. The spin indices run from $-j$ to j, and we have introduced the notation

$$\Gamma_{\alpha\beta} \equiv f^\dagger_\alpha f_\beta = |f^1:\alpha\rangle\langle f^1:\beta|$$

Notice that the charge $Q = n_f$ of the $f-$electron, normally taken to be unity, is conserved by the spin-exchange interaction in this Hamiltonian.

To get an idea of how the Kondo effect is modified by the larger degeneracy, consider the renormalization of the interaction, which is given by the diagram

$$J_{eff}(D') = \quad + \quad$$



$$= J + NJ^2\rho \ln\left(\frac{D}{D'}\right) \tag{16.7}$$

(where the cross on the intermediate conduction electron state indicates that all states with energy $|\epsilon_k| \in [D', D]$ are integrate over). From this result, we see that $\beta(g) = \partial g(D)/\partial \ln D = -Ng^2$, where $g = J\rho$ has an $N-$ fold enhancement, derived from the N intermediate hole states. A more extensive calculation shows that the beta function to third order takes the form

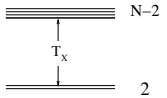
$$\beta(g) = -Ng^2 + Ng^3. \tag{16.8}$$

This then leads to the Kondo temperature

$$T_K = D(NJ\rho)^{\frac{1}{N}} \exp\left[-\frac{1}{NJ\rho}\right]$$

so that large degeneracy enhances the Kondo temperature in the exponential factor. By contrast, the RKKY interaction strength is given by $T_{RKKY} \sim J^2\rho$, and it does not involve any N fold enhancement factors, thus in systems with large spin degeneracy, the enhancement of the Kondo temperature favors the formation of the heavy fermion ground-state.

In practice, rare-earth ions are exposed to the crystal fields of their host, which splits the $N = 2j + 1$ fold degeneracy into many multiplets. Even in this case, the large degeneracy is helpful, because the crystal field splitting is small compared with the band-width. At energies D' large compared with the crystal field splitting T_x, $D' >> T_x$, the physics is that of an N fold degenerate ion, whereas at energies D' small compared with the crystal field splitting, the physics is typically that of a Kramers doublet, i.e.



$$\frac{\partial g}{\partial \ln D} = \begin{cases} -Ng^2 & (D >> T_x) \\ -2g^2 & (D << T_x) \end{cases} \tag{16.9}$$

from which we see that at low energy scales, the leading order renormalization of g is given by

$$\frac{1}{g(D')} = \frac{1}{g_o} - N\ln\left(\frac{D}{T_x}\right) - 2\ln\left(\frac{T_x}{D'}\right)$$

where the first logarithm describes the high energy screening with spin degeneracy N, and the second logarithm describes the low-energy screening, with spin degeneracy 2. This expression is ~ 0 when $D' \sim T_K^*$, the Kondo temperature, so that

$$0 = \frac{1}{g_o} - N\ln\left(\frac{D}{T_x}\right) - 2\ln\left(\frac{T_x}{T_K^*}\right)$$

from which we deduce that the renormalized Kondo temperature has the form[7]

$$T_K^* = D\exp\left(-\frac{1}{2J_o\rho}\right)\left(\frac{D}{T_x}\right)^{\frac{N}{2}-1}.$$

Here the first term is the expression for the Kondo temperature of a spin 1/2 Kondo model. The second term captures the enhancement of the Kondo temperature coming from the renormalization effects at scales larger than the crystal field splitting. Suppose $T_x \sim 100K$, and $D \sim 1000K$, and $N = 6$, then the enhancement factor is order 100. This effect enhances the Kondo temperature of rare earth heavy fermion systems to values that are indeed, up to a hundred times bigger than those in transition metal systems. This is the simple reason why heavy fermion behavior is rare in transition metal systems. [**?**] In short- spin-orbit coupling, even in the presence of crystal fields, substantially enhances the Kondo temperature.

The exhaustion problem

At temperatures $T \leq T_K$, a local moment is "screened" by conduction electrons. What does this actually mean? The conventional view of the Kondo effect interprets it in terms of the formation of a "magnetic screening cloud" around the local moment. According to the screening cloud picture, the electrons which magnetically screen each local moment are confined within an energy range of order $\delta\epsilon \sim T_K$ around the Fermi surface, giving rise to a spatially extended screening cloud of dimension $l = v_F/T_K \sim a\frac{\epsilon_F}{T_K}$, where a is a lattice constant and ϵ_F is the Fermi temperature. In a typical heavy fermion system, this length would extend over hundreds of lattice constants. This leads to the following two dilemmas

1. It suggests that when the density of magnetic ions is greater than $\rho \sim 1/l^3$, the screening clouds will interfere. Experimentally no such interference is observed, and features of single ion Kondo behavior are seen at much higher densities.

2. " The exhaustion paradox" The number of "screening"electrons per unit cell within energy T_K of the Fermi surface roughly T_K/W, where W is the bandwidth, so there would never be enough low energy electrons to screen a dense array of local moments.

In this lecture I shall argue that the screening cloud picture of the Kondo effect is conceptually incorrect. Although the Kondo effect does involve a binding of local moments to electrons, the binding process takes place between the local moment and high energy electrons , spanning decades of energy from the Kondo temperature up to the band-width. (Fig. 16.5) I shall argue that the key physics of the Kondo effect, both in the dilute impurity and dense Kondo lattice, involves

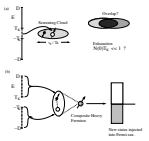


Figure 16.5: Contrasting (a) the "screening cloud" picture of the Kondo effect with (b) the composite fermion picture. In (a), low energy electrons form the Kondo singlet, leading to the exhaustion problem. In (b) the composite heavy electron is a highly localized bound-state between local moments and high energy electrons which injects new electronic states into the conduction sea at the chemical potential. Hybridization of these states with conduction electrons produces a singlet ground-state, forming a Kondo resonance in the single impurity, and a coherent heavy electron band in the Kondo lattice.

the formation of a composite heavy fermion formed by binding electrons on logarithmically large energy scales out to the band-width. These new electronic states are injected into the conduction electron sea near the Fermi energy. For a single impurity, this leads to a single isolated resonance. In the lattice, the presence of a new multiplet of fermionic states at each site leads to the formation of a coherent heavy electron band with an expanded Fermi surface. (16.5)

16.1.1 Large N Approach

We shall now solve the Kondo model, both the single impurity and the lattice, in the large N limit. In the early eighties, Anderson[**?**] pointed out that the large spin degeneracy $N = 2j+1$ furnishes a small parameter $1/N$ which might be used to develop a controlled expansion about the limit $N \to \infty$. Anderson's observation immediately provided a new tool for examining the heavy fermion problem: the so called "large N expansion". [8].

The basic idea behind the large N expansion, is to take a limit where every term in the Hamiltonian grows extensively with N. In this limit, quantum fluctuations in intensive variables, such as the electron density, become smaller and smaller, scaling as $1/N$, and in this sense,

$$\frac{1}{N} \sim \hbar_{eff}$$

behaves as an effective Planck's constant for the theory. In this sense, a large N expansion is a semi-classical treatment of the quantum mechanics, but instead of expanding around $\hbar = 0$, one can obtain new, non trivial results by expanding around the non trivial solvable limit $\frac{1}{N} = 0$. For the Kondo model, we are lucky, because the important physics of the Kondo effect is already captured by the large N limit as we shall now see.

Our model for a Kondo lattice or an ensemble of Kondo impurities localized at sites j is

$$H = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + \sum_j H_I(j) \tag{16.10}$$

where

$$H_I(j) = \frac{J}{N}\Gamma_{\alpha\beta}(j)\psi^\dagger{}_\beta(j)\psi_\alpha(j)$$

is the interaction Hamiltonian between the local moment and conduction sea. Here, the spin of the local moment at site j is represented using pseudo-fermions

$$\Gamma_{\alpha\beta}(j) = f^\dagger{}_{j\alpha}f_{j\beta},$$

and

$$\psi^\dagger{}_\alpha(j) = \sum_{\vec{k}} c^\dagger{}_{\vec{k}\alpha}e^{-i\vec{k}\cdot\vec{R}_j}$$

creates an electron localized at site j.

There are a number of technical points about this model that need to be discussed:

- **The spherical cow approximation**. For simplicity, we assume that electrons have a spin degeneracy $N = 2j + 1$. This is a theorists' idealization- a "spherical cow approximation" which can only be strictly justified for a single impurity. Nevertheless, the basic properties of this toy model allow us to understand how the Kondo effect works in a Kondo lattice. With an N-fold conduction electron degeneracy, it is clear that the Kinetic energy will grow as $O(N)$.

- **Scaling the interaction.** Now the interaction part of the Hamiltonian $H_I(j)$ involves two sums over the spin variables, giving rise to a contribution that scales as $O(N^2)$. To ensure that the interaction energy grows extensively with N, we need to scale the coupling constant as $O(1/N)$.

- **Constraint** $n_f = Q$. Irreducible representations of the rotation group SU (N) require that the number of $f-$electrons at a given site is constrained to equal to $n_f = Q$. In the large N limit, it is sufficient to apply this constraint on the average $\langle n_f\rangle = Q$, though at finite N a time dependent Lagrange multiplier coupled to the difference $n_f - Q$ is required to enforce the constraint dynamically. With Q $f-$electrons, the spin operators $\Gamma_{ab} = f^\dagger{}_a f_b$ provide an irreducible *antisymmetric* representation of $SU(N)$ that is described by column Young Tableau with Q boxes. As N is made large, we need to ensure that $q = Q/N$ remains fixed, so that $Q \sim O(N)$ is an extensive variable. Thus, for instance, if we are interested in $N = 2$, this corresponds to $q = n_f/N = \frac{1}{2}$. We may obtain insight into this case by considering the large N limit with $q = 1/2$.

The next step in the large N limit is to carry out a "Hubbard Stratonovich" transformation on the interaction. We first write

$$H_I(j) = -\frac{J}{N}\left(\psi^\dagger{}_{j\beta}f_{j\beta}\right)\left(f^\dagger{}_{j\alpha}\psi_{j\alpha}\right),$$

with a summation convention on the spin indices. We now factorize this[9, 10] as

$$H_I(j) \to H_I[V,j] = \bar{V}_j\left(\psi^\dagger{}_{j\alpha}f_{j\alpha}\right) + \left(f^\dagger{}_{j\alpha}\psi_{j\alpha}\right)V_j + N\frac{\bar{V}_jV_j}{J}$$

This is an exact transformation, provided the hybridization variables $V_j(\tau)$ are regarded as fluctuating variables inside a path integral, so formally,

$$Z = \int \mathcal{D}[V,\lambda]\overbrace{\mathrm{Tr}[T\exp\left[-\int_0^\beta H[V,\lambda]\right]]}^{Z[\lambda,V]} \tag{16.11}$$

where

$$H[V,\lambda] = \sum_{\vec{k}\sigma}\epsilon_{\vec{k}}c^\dagger{}_{\vec{k}\sigma}c_{\vec{k}\sigma} + \sum_j\left(H_I[V_j,j] + \lambda_j[n_f(j) - Q]\right), \tag{16.12}$$

is exact. In this expression, $\mathcal{D}[V,\lambda]$ denotes a path integral over all possible time-dependences of V_j and $\lambda_j(\tau)$, and T denotes time ordering. The important point for our discussion here however, is that in the large N limit, the Hamiltonian entering into this path integral grows extensively with N, so that we may write the partition function in the form

$$Z = \int \mathcal{D}[V,\lambda]\mathrm{Tr}[T\exp\left[-N\int_0^\beta \mathcal{H}[V,\lambda]\right] \tag{16.13}$$

where $\mathcal{H}[V,\lambda] = \frac{1}{N}H[V,\lambda] \sim O(1)$ is an intensive variable in N. The appearance of a large factor N in the exponential means that this path integral becomes dominated by its saddle points in the large N limit- i.e, if we choose

$$V_j = V_o, \qquad \lambda_j = \lambda_o$$

where the saddle point values V_o and λ_o are chosen so that

$$\left.\frac{\partial \ln Z[V,\lambda]}{\partial V}\right|_{V_j=V_o,\lambda_j=\lambda_o} = \left.\frac{\partial \ln Z[V,\lambda]}{\partial \lambda}\right|_{V_j=V_o,\lambda_j=\lambda_o} = 0$$

then in the large N limit,

$$Z = \mathrm{Tr}e^{-\beta H[V_o,\lambda_o]}$$

In this way, we have converted the problem to a mean-field theory, in which the fluctuating variables $V_j(\tau)$ and $\lambda_j(\tau)$ are replaced by their saddle-point values. Our mean-field Hamiltonian is then

$$H_{MFT} = \sum_{\vec{k}\sigma}\epsilon_{\vec{k}}c^\dagger{}_{\vec{k}\sigma}c_{\vec{k}\sigma} + \sum_{j,\alpha}\left(f^\dagger{}_{j\alpha}\psi_{j\alpha}V_o + \bar{V}_o\psi^\dagger{}_{j\beta}f_{j\beta} + \lambda_o f^\dagger{}_{j\alpha}f_{j\alpha}\right) + Nn\left(\frac{\bar{V}_oV_o}{J} - \lambda_o q\right),$$

where n is the number of sites in the lattice. We shall now illustrate the use of this mean-field theory in two cases- the Kondo impurity, and the Kondo lattice. In the former, there is just one site; in the latter, translational invariance permits us to set $V_j = V_o$ at every site, and for convenience we shall choose this value to be real.

16.1.2 Mean-field theory of the Kondo impurity

Diagonalization of MF Hamiltonian

The Kondo effect is at heart, the formation of a many body resonance. To understand this phenomenon at its conceptually simplest, we begin with the impurity model. We shall begin by writing down the mean-field Hamiltonian for a single Kondo ion

$$H = \sum_{k\sigma} \epsilon_k c^\dagger{}_{k\sigma} c_{k\sigma} + \sum_{k\sigma} V[c^\dagger{}_{k\sigma} f_\sigma + f^\dagger{}_\sigma c_{k\sigma}] + \lambda \sum_\sigma n_{f\sigma} - \lambda Q + \frac{NV^2}{J} \tag{16.14}$$

By making a mean-field approximation, we have reduced the problem to one of a self-consistently determined resonant level model. Now, suppose we diagonalize this Hamiltonian, writing it in the form

$$H = \sum_{\gamma\sigma} E_\gamma a^\dagger{}_{\gamma\sigma} a_{\gamma\sigma} + \frac{NV^2}{J} - \lambda Q \tag{16.15}$$

where the "quasiparticle operators" α_γ are related via a unitary transformation to the original operators

$$a^\dagger{}_{\gamma\sigma} = \sum_k \alpha_k c^\dagger{}_{k\sigma} + \beta f^\dagger{}_\sigma. \tag{16.16}$$

commuting $a^\dagger{}_{\gamma\sigma}$ with H, we obtain

$$[H,\ a^\dagger{}_{\gamma\sigma}] = E_\gamma a^\dagger \tag{16.17}$$

Expanding the right and left-hand side of (16.17) in terms of (16.16) and (16.14), we obtain,

$$\begin{aligned} (E_\gamma - \epsilon_k)\alpha_k - V\beta &= 0 \\ -V\sum_k \alpha_k + (E_\gamma - \lambda)\beta &= 0 \end{aligned} \tag{16.18}$$

Solving for α_k using the first equation, and substituting into the second equation, we obtain

$$E_\gamma - \lambda - \sum_k \frac{V^2}{E_\gamma - \epsilon_k} = 0 \tag{16.19}$$

We could have equally well obtained these eigenvalue equations by noting the electron eigenvalues E_γ must correspond to the poles of the f-Green function, $G_f(E_\gamma)^{-1} = 0$, where from an earlier subsection,

$$G_f^{-1}(\omega) = \left[\omega - \lambda - \sum_k \frac{V^2}{\omega - \epsilon_k}\right] \tag{16.20}$$

Either way, the one-particle excitation energies E_γ must satisfy

$$E_\gamma = \lambda + \sum_k \frac{V_o^2}{E_\gamma - \epsilon_k} \tag{16.21}$$

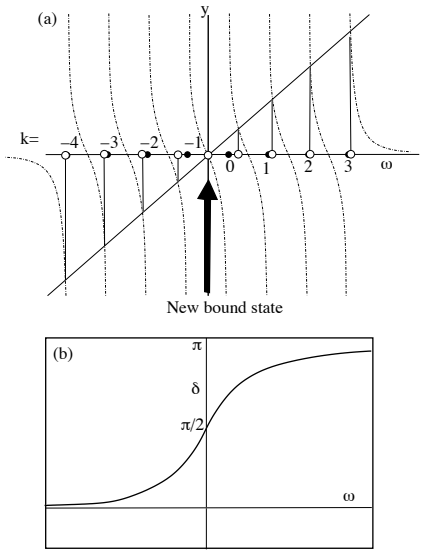


Figure 16.6: (a) Graphical solution of the equation $y = -\sum_k \frac{V^2}{y-\epsilon_k}$, for eight equally spaced conduction electron energies. Notice how the introduction of a new bound-state at $y = 0$ displaces electron band-states both up and down in energy. In this way, the Kondo effect injects new bound-state fermion states into the conduction sea. (b) Energy dependence of the scattering phase shift.

The solutions of this eigenvalue equation are illustrated graphically in Fig. (16.6). Suppose the energies of the conduction sea are given by the $2M$ discrete values

$$\epsilon_k = (k + \frac{1}{2})\Delta\epsilon, \qquad k \in \{-M, \ldots, M-1\}$$

Suppose we restrict our attention to the particle-hole case when the f-state is exactly half filled, i.e. when $Q = N/2$. In this situation, $\lambda = 0$. We see that one solution to the eigenvalue equation corresponds to $E_\gamma = 0$. The original band-electron energies are now displaced to both lower and higher energies, forming a band of $2M + 1$ eigenvalues. Clearly, the effect of the hybridization is to inject one new fermionic eigenstate into the band. Notice however, that the electron states are displaced symmetrically either-side of the new bound-state at $E_\gamma = 0$.

Each new eigenvalue is shifted relative to the original conduction electron energy by an amount

of order $\Delta\epsilon$. Let us write

$$E_\gamma = \epsilon_\gamma - \Delta\epsilon\frac{\delta_\gamma}{\pi}$$

where $\delta \in [0,\pi]$ is called the "phase shift". Substituting this into the eigenvalue equation, we obtain

$$E_\gamma = \lambda + \sum_{n=\gamma+1-M}^{\gamma+M} \frac{V_{o^2}}{\Delta\epsilon(n-\frac{\delta}{\pi})}$$

Now if M is large, we can replace the sum over states in the above equation by an unbounded sum

$$E_\gamma = \lambda + \frac{V_o^2}{\Delta\epsilon}\sum_{n=-\infty}^{\infty}\frac{1}{(n-\frac{\delta}{\pi})}$$

Using contour integration methods, one can readily show that

$$\sum_{n=-\infty}^{\infty}\frac{1}{(n-\frac{\delta}{\pi})} = -\pi\cot\delta$$

so that the phase shift is given by $\delta_\gamma = \delta(E_\gamma)$, where

$$\tan\delta[\epsilon] = \frac{\pi\rho V_o^2}{\lambda-\epsilon}$$

where we have replaced $\rho = \frac{1}{\Delta\epsilon}$ as the density of conduction electron states. This can also be written

$$\delta(\epsilon) = \tan^{-1}\left[\frac{\Delta}{\lambda-\epsilon}\right] = \mathrm{Im}\ln[\lambda+i\Delta-\epsilon] \tag{16.22}$$

where $\Delta = \pi\rho V_o^2$ is the width of the resonant level induced by the Kondo effect. Notice that for $\lambda = 0$, $\delta = \pi/2$ at the Fermi energy.

- The phase shift varies from $\delta = 0$ at $E_\gamma = -\infty$ to $\delta = \pi$ at $E_\gamma = \infty$, passing through $\delta = \pi/2$ at the Fermi energy.
- An extra state has been inserted into the band, squeezing the original electron states both down and up in energy to accommodate the additional state: states beneath the Fermi sea are pushed downwards, whereas states above the Fermi energy are pushed upwards. From the relation

  $$E_\gamma = \epsilon_\gamma - \frac{\Delta\epsilon}{\pi}\delta(E_\gamma)$$

  we deduce that

  $$\begin{aligned}\frac{d\epsilon}{dE} &= 1 + \frac{\Delta\epsilon}{\pi}\frac{d\delta(E)}{dE}\\ &= 1 + \frac{1}{\pi\rho}\frac{d\delta(E)}{dE}\end{aligned} \tag{16.23}$$

where $\rho = 1/\Delta\epsilon$ is the density of states in the continuum. The new density of states $\rho^*(E)$is given by $\rho^*(E)dE = \rho d\epsilon$, so that

$$\rho^*(E) = \rho(0)\frac{d\epsilon}{dE} = \rho + \rho_i(E) \tag{16.24}$$

where

$$\rho_i(E) = \frac{1}{\pi}\frac{d\delta(E)}{dE} = \frac{1}{\pi}\frac{\Delta^2}{(E-\lambda)^2+\Delta^2} \tag{16.25}$$

corresponds to the enhancement of the conduction electron density of states due to injection of resonant bound-state.

Minimization of Free energy

With these results, let us now calculate the Free energy and minimize it to self-consistently evaluate λ and Δ. The Free energy is given by

$$F = -NT\sum_\gamma \ln[1+e^{-\beta E_\gamma}] - \lambda Q + \frac{NV_o^2}{J}. \tag{16.26}$$

In the continuum limit, where $\epsilon \to 0$, we can use the relation $E_\gamma = \epsilon_\gamma - \Delta\epsilon\frac{\delta}{\pi}$ to write

$$\begin{aligned}-T\ln[1+e^{-\beta E_\gamma}] &= -T\ln[1+e^{-\beta(\epsilon_\gamma-\Delta\epsilon\frac{\delta}{\pi})}]\\ &= \overbrace{-T\ln[1+e^{-\beta\epsilon_\gamma}]}^{\to F_0} - \frac{\Delta\epsilon}{\pi}\delta(\epsilon_\gamma)f(\epsilon_\gamma)\end{aligned} \tag{16.27}$$

where $f(x) = 1/(e^{\beta x}+1)$ is the Fermi function. The first term in (16.27) is the Free energy associated with a state in the continuum. The second term results from the displacement of continuum states due to the injection of a resonance into the continuum. Inserting this result into (16.26), we obtain

$$\begin{aligned}F &= F_0 - N\sum_\gamma \frac{\Delta\epsilon}{\pi}\delta(\epsilon_\gamma)f(\epsilon_\gamma) - \lambda Q + \frac{NV_o^2}{J}\\ &= F_0 - N\int_{-\infty}^{\infty}\frac{d\epsilon}{\pi}f(\epsilon)\delta(\epsilon) - \lambda Q + \frac{NV_o^2}{J}\end{aligned} \tag{16.28}$$

The shift in the Free energy due to the Kondo effect is then

$$\Delta F = -N\int_{-\infty}^{\infty}\frac{d\epsilon}{\pi}f(\epsilon)\mathrm{Im}\ln[\zeta-\epsilon] - \lambda Q + \frac{N\Delta}{\pi J\rho} \tag{16.29}$$

where we have introduced $\zeta = \lambda + i\Delta$. This integral can be done at finite temperature, but for simplicity, let us carry it out at $T = 0$, when the Fermi function is just at step function, $f(x) = \theta(-x)$. This gives

$$\Delta E = \frac{N}{\pi}\mathrm{Im}\left[(\zeta-\epsilon)\ln\left[\frac{\zeta-\epsilon}{e}\right]\right]_{-D}^{0} - \lambda Q + \frac{N\Delta}{\pi J\rho}$$

$$= \frac{N}{\pi}\mathrm{Im}\Big[\zeta \ln\Big[\frac{\zeta}{eD}\Big] - D\ln\Big[\frac{D}{e}\Big]\Big] - \lambda Q + \frac{N\Delta}{\pi J\rho} \tag{16.30}$$

where we have expanded $(\zeta + D)\ln\left[\frac{D+\zeta}{e}\right] \to D\ln\left[\frac{D}{e}\right] + \zeta \ln D$ to obtain the second line. We can further simplify this expression by noting that

$$-\lambda Q + \frac{N\Delta}{\pi J\rho} = -\frac{N}{\pi}\mathrm{Im}\Big[\zeta \ln\Big[e^{-\frac{1}{\rho J}+i\pi q}\Big]\Big] \tag{16.31}$$

where $q = Q/N$. With this simplification, the shift in the ground-state energy due to the Kondo effect is

$$\Delta E = \frac{N}{\pi}\mathrm{Im}\Big[\zeta \ln\Big[\frac{\zeta}{eT_K e^{i\pi q}}\Big]\Big] \tag{16.32}$$

where we have dropped the constant term and introduced the Kondo temperature $T_K = De^{-\frac{1}{J\rho}}$. The stationary point $\partial E/\partial\zeta = 0$ is given by

$$\zeta = \lambda + i\Delta = T_K e^{i\pi q} \qquad \begin{cases} T_K &= \sqrt{\lambda^2+\Delta^2} \\ \tan(\pi q) &= \frac{\Delta}{\lambda} \end{cases}$$

Notice that

- The phase shift $\delta = \pi q$ is the same in each spin scattering channel, reflecting the singlet nature of the ground state. The relationship between the filling of the resonance and the phase shift $Q = \sum_\sigma \frac{\delta_\sigma}{\pi} = N\frac{\delta}{\pi}$ is nothing more than Friedel's sum rule.
- The energy is stationary with respect to small variations in λ and Δ. It is only a local minimum once the condition $\partial E/\partial\lambda$, corresponding to the constraint $\langle \hat{n}_f\rangle = Q$, or $\lambda = \Delta\cot(\pi q)$ is imposed. It is instructive to study the energy for the special case $q = \frac{1}{2}$, $\lambda = 0$ which is physically closest to the $S = 1/2$, $N = 2$ case. In this case, the energy takes the simplified form

  $$\Delta E = \frac{N}{\pi}\Big[\Delta \ln\Big[\frac{\Delta}{eT_K}\Big]\Big] \tag{16.33}$$

  Plotted as a function of V, this is the classic "Mexican Hat" potential, with a minimum where $\partial E/\partial V = 0$ at $\Delta = \pi\rho|V|^2 = T_K$. (Fig. 16.7)
- According to (16.24), the enhancement of the density of states at the Fermi energy is

  $$\begin{aligned}\rho^*(0) &= \rho + \frac{\Delta}{\pi(\Delta^2+\lambda^2)} \\ &= \rho + \frac{\sin^2(\pi q)}{\pi T_K}\end{aligned} \tag{16.34}$$

  per spin channel. When the temperature is changed or a magnetic field introduced, one can neglect changes in Δ and λ, since the Free energy is stationary. This implies that in the large N limit, the susceptibility and linear specific heat are those of a non-interacting resonance of

width Δ. The change in linear specific heat $\Delta C_V = \Delta\gamma T$ and the change in the paramagnetic susceptibility $\Delta\chi$ are given by

$$\begin{aligned}\Delta\gamma &= \Big[\frac{N\pi^2 k_B^2}{3}\Big]\rho_i(0) = \Big[\frac{N\pi^2 k_B^2}{3}\Big]\frac{\sin^2(\pi q)}{\pi T_K} \\ \Delta\chi &= \Big[N\frac{j(j+1)(g\mu_B)^2}{3}\Big]\rho_i(0) = \Big[N\frac{j(j+1)(g\mu_B)^2}{3}\Big]\frac{\sin^2(\pi q)}{\pi T_K}\end{aligned} \tag{16.35}$$

Notice how it is the Kondo temperature that determines the size of these two quantities. The dimensionless "Wilson" ratio of these two quantities is

$$W = \Big[\frac{(\pi k_B)^2}{(g\mu_B)^2 j(j+1)}\Big]\frac{\Delta\chi}{\Delta\gamma} = 1$$

At finite N, fluctuations in the mean-field theory can no longer be ignored. These fluctuations induce interactions amongst the quasiparticles, and the Wilson ratio becomes

$$W = \frac{1}{1-\frac{1}{N}}.$$

The dimensionless Wilson ratio of a large variety of heavy electron materials lies remarkably close to this value.

16.1.3 Gauge invariance and the composite nature of the $f-$electron

We now discuss the nature of the $f-$electron. In particular, we shall discuss how

- the $f-$electron is actually a composite object, formed from the binding of high-energy conduction electrons to the local moment.
- although the broken symmetry associated with the large N mean-field theory does not persist to finite N, the phase stiffness associated with the mean-field theory continues to finite N. This phase stiffness is responsible for the charge of the composite f electron.

Composite nature of the heavy $f-$electron

Let us begin by discussing the composite structure of the $f-$electron. In real materials, the Kondo effect we have described involves spins formed from localized f- or d-electrons. Though it is tempting to associate the composite $f-$electron in the Kondo effect with the the $f-$electron locked inside the local moment, we should also bear in mind that the Kondo effect could have occurred equally well with a nuclear spin! Nuclear spins do couple antiferromagnetically with a conduction electron, but the coupling is far too small for an observable nuclear Kondo effect. Nevertheless, we could conduct a thought experiment where a nuclear spin is coupled to conduction electrons via a strong antiferromagnetic coupling. In this case, a resonant bound-state would also form from the nuclear spin. The composite bound-state formed in the Kondo effect clearly does not depend on the origin of the spin partaking in the Kondo effect.

There are some useful analogies between the formation of the composite $f-$electron in the Kondo problem and the formation of Cooper pairs in superconductivity, which we shall try to draw upon. One of the best examples of a composite bound-state is the Cooper pair. Inside a superconductor, pairs of electrons behave as composite bosonic particles. One of the signatures of pair formation, is the fact that Cooper pairs of electron operators behave as a single composite at low energies,

$$\psi_\uparrow(x)\psi_\downarrow(x') \equiv F(x-x')$$

The Cooper pair operator is a boson, and it behaves as a c-number because the Cooper pairs condense. The Cooper pair wavefunction is extremely extended in space, extending out to distances of order $\xi \sim v_F/T_c$. A similar phenomenon takes place in the Kondo effect, but here the bound-state is a *fermion* and it does not condense For the Kondo effect the fermionic composite $(\vec{\sigma}\cdot\vec{S}(x))_{\alpha\beta}\psi_\beta(x)$ behaves as a single charged electron operator. The analogy between superconductivity and the Kondo effect involves the temporal correlation between spin-flips of the conduction sea and spin-flips of the local moment, so that at low energies

$$[\vec{\sigma}_{\alpha\beta}\cdot\vec{S}(t)]\psi_\beta(t') \sim \Delta(t-t')f_\alpha(t').$$

The function $\Delta(t-t')$ is the analog of the Cooper pair wavefunction, and it extends out to times $\tau_K \sim \hbar/T_K$.

To see this in a more detailed fashion, consider how the interaction term behaves. In the path integral we factorize the interaction as follows

$$H_I = \frac{J}{N}\psi^\dagger{}_\beta\Gamma_{\alpha\beta}\psi_\alpha \rightarrow \bar{V}\left(\psi^\dagger{}_\alpha f_\alpha\right) + \left(f^\dagger{}_\alpha\psi_\alpha\right)V + N\frac{\bar{V}V}{J}$$

By comparing these two terms, we see that the composite operator $\Gamma_{\alpha\beta}(j)\psi_\alpha(j)$ behaves as a single fermi field:

$$\frac{1}{N}\Gamma_{\alpha\beta}(t)\psi_\alpha(t) \rightarrow \left(\frac{\bar{V}}{J}\right)f_\alpha(t)$$

Evidently, a localized conduction electron is bound to a spin-flip of the local moment at the same site, creating a new independent fermionic excitation. The correlated action of adding a conduction electron with a simultaneous spin flip of the local moment at the same site creates a composite $f-$electron.

It is worth noting that this fermionic object only hybridizes with conduction electrons at a single point: it is thus local in space.

Let us now try to decompose the composite fermion in terms of the electrons that contribute to the bound-state amplitude. We start by writing the local moment in the fermionic representation, [3]

$$\frac{1}{N}\Gamma_{\alpha\beta}\psi_\alpha = -\frac{1}{N}f^\dagger{}_\beta\psi_\alpha f_\alpha \rightarrow -\frac{1}{N}\langle f^\dagger{}_\beta\psi_\beta\rangle f_\beta$$

[3] Important and subtle point: The emergence of a composite fermion does not depend on a fermionic representation of the spin. The fermionic representation for the spin is simply the most convenient because it naturally furnishes us with an operator in the theory that represents the composite bound-state.

where we have replaced the bilinear product between the conduction and $f-$electron by its expectation value. We can evaluate this "bound-state amplitude" from the corresponding Green-function

$$\begin{aligned} -\frac{V}{J} = \frac{1}{N}\langle f^\dagger{}_\beta\psi_\beta\rangle &= \int\frac{d\omega}{\pi}f(\omega)\mathrm{Im}G_{\psi f}(\omega-i\delta) \\ &= V_o\int f(\omega)\frac{d\omega}{\pi}\mathrm{Im}\left[\sum_k \frac{1}{\omega-\epsilon_k-i\delta}\frac{1}{\omega-i\Delta}\right] \end{aligned} \tag{16.36}$$

where we have chosen the half-filled case $Q/N = 1/2$, $\lambda = 0$. In the large band-width limit, the main contribution to this integral is obtained by neglecting the principal part of the conduction electron propagator $1/(\omega-\epsilon_k-i\delta) \rightarrow i\pi\delta(\omega-\epsilon_k)$, so that

$$\frac{1}{N}\langle f^\dagger{}_\beta\psi_\beta\rangle = \sum_k f(\epsilon_k)\left(\frac{\epsilon_k}{\epsilon_k^2+\Delta^2}\right) \tag{16.37}$$

From this expression, we can see that the contribution of a given k state in the Fermi sea to the bound-state amplitude is given by

$$\frac{1}{N}\langle f^\dagger{}_\beta c_{k\beta}\rangle = f(\epsilon_k)\left(\frac{\epsilon_k}{\epsilon_k^2+\Delta^2}\right)$$

This function decays with the inverse of the energy, right out to the band-width. Indeed, if we breakdown the contribution to the overall bound-state amplitude, we see that each decade of energy counts equally. Let us take $T = 0$ and divide the band on a logarithmic scale into n equal parts, where the ratio of the lower and upper energies is $s > 1$, then

$$\begin{aligned} \frac{V_o}{J} &= \rho V_o\int_{-D}^{0}d\epsilon\frac{-\epsilon}{\epsilon^2+\Delta^2} \sim \rho V_o\int_\Delta^D d\epsilon\frac{1}{\epsilon} \\ &= \rho V_o\left\{\int_{D/s}^{D} + \int_{D/s^2}^{D/s} + \ldots\int_{D/s^n}^{D/s^{n-1}} + \int_\Delta^{D/s^n}\right\}\frac{d\epsilon}{\epsilon} \\ &= \rho V_0\left\{\ln s + \ln s + \ldots\ln s + \ln\frac{Ds^{-n}}{\Delta}\right\} \end{aligned} \tag{16.38}$$

This demonstrates that the composite bound-state involves electrons on spread out over decades of energy out to the band-width. If we complete the integral, we find that

$$\frac{V_o}{J} = \rho V_o\ln\frac{D}{\Delta} \Rightarrow \Delta = De^{-\frac{1}{J\rho}} = T_K$$

as expected from the minimization of the energy. Another way of presenting this discussion, is to write the composite bound-state in the time-domain, as

$$\frac{1}{N}\Gamma_{\alpha\beta}(t')\psi_\alpha(t) \rightarrow \Delta(t-t')f_\alpha(t') \tag{16.39}$$

where now

$$\Delta(t-t') = \frac{1}{N}\langle f_\beta^\dagger(t)\psi_\beta(t')\rangle$$

This is the direct analog of Cooper pair bound-state wavefunction, except that the relevant variable is time, rather than space. If one evaluates the function $\Delta(t)$ at a finite t, we find that

$$\Delta(t-t') = \sum_k f(\epsilon_k)\left(\frac{\epsilon_k}{\epsilon_k^2+\Delta^2}\right)e^{-i\epsilon_k(t-t')}$$

Heuristically, the finite time cuts off the energy integral over the Fermi surface at an energy of order $\hbar/t$, so that

$$\Delta(t) \sim \begin{cases} \rho V_o \ln\left(\frac{Dt}{\hbar}\right) & (t << \hbar/T_K) \\ \rho V_o \ln\left(\frac{D}{T_K}\right) & (t >> \hbar/T_K) \end{cases}$$

emphasizing the fact that the Kondo effect involves a correlation between the spin-flips of the conduction sea and the local moment over decades of time scales from the the inverse band-width up to the Kondo time $\hbar/T_K$.

From these discussions, we see that the Kondo effect is

- entirely localized in space.
- extremely non-local in time and energy.

This picture of the Kondo effect as a temporal, rather than a spatial bound-state is vital if we are to understand the extension of the Kondo effect from the single impurity to the lattice.

Gauge invariance and the charge of the $f-$electron

One of the interesting points to emerge from the mean-field theory is that the energy of mean-field theory does not depend on the phase of the bound-state amplitude $V = |V|e^{i\theta}$. This is analogous to the gauge invariance in superconductivity, which derives from the conservation of the total electronic charge. Here, gauge invariance arises because there are no charge fluctuations at the site of the local moment, a fact encoded by the conservation of the total f-charge Q. Let us look at the full Lagrangian for the $f-$electron and interaction term

$$\begin{aligned} \mathcal{L}_I &= {f_\sigma}^\dagger(i\partial_t - \lambda)f_\sigma - H_I \\ H_I &= \bar{V}\left({\psi^\dagger}_\alpha f_\alpha\right) + \left({f^\dagger}_\alpha \psi_\alpha\right)V + N\frac{\bar{V}V}{J} \end{aligned} \tag{16.40}$$

This is invariant under the "Read-Newns"[10] transformation

$$\begin{aligned} f &\rightarrow f e^{i\phi}, \\ V &\rightarrow V e^{i\phi}, \qquad (\theta \rightarrow \theta + \phi), \\ \lambda &\rightarrow \lambda + \frac{\partial\phi}{\partial t}. \end{aligned} \tag{16.41}$$

where the last relation arises from a consideration of the gauge invariance of the dynamic part $f^\dagger(i\partial_t - \lambda)f$ of the Lagrangian. Now if $V(t) = |V(t)|e^{\theta(t)}$, where $r(t)$ is real, Read and Newns observed that by making the gauge choice $\phi(t) = -\theta(t)$, the resulting $V = |V|e^{i(\theta+\phi)} = |V|$ is real.

In this way, once the Kondo effect takes place the phase of $V = |V|e^{i\theta}$ is dynamically absorbed into the constraint field λ : effectively $\lambda \equiv \partial_t\phi$ represents the phase precession rate of the hybridization field. The absorption of the phase of an order parameter into a dynamical gauge field is called the "Anderson Higg's" mechanism.[**?**] By this mechanism, once the Kondo effect takes place, V behaves as a real, and hence neutral object under gauge transformations, this in turn implies that the composite $f-$electron has to transform under real electromagnetic gauge transformations, in other words the Anderson Higgs effect in the Kondo problem endows the composite $f-$electron with charge.

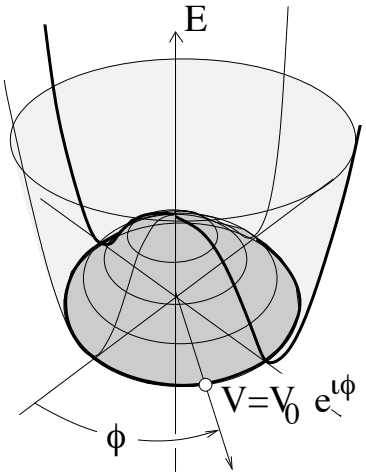


Figure 16.7: "Mexican Hat Potential" which determines minimum of Free energy, and self-consistently determines the width of the Kondo resonance. The Free energy displays this form provided the constraint $\partial F/\partial\lambda = \langle n_f\rangle - Q = 0$ is imposed.

There is a paradox here, for in the Kondo effect, there can actually be no true broken symmetry, since we are dealing with a system where the number of local degrees of freedom is finite. Nevertheless, the phase ϕ does develop a stiffness- a stiffness against variation in time, and the order parameter consequently develops infinite range correlations in time. There is a direct analogy between the spatial phase stiffness of a superconductor and the temporal phase stiffness in the Kondo effect. In superconductivity, the energy depends on spatial derivatives of the phase

$$E \propto \frac{\rho_s}{2}(\nabla\phi - 2e\vec{A})^2 \Rightarrow \frac{1}{\lambda_L}^2 \propto \rho_s$$

(where we have set $\hbar = 1$.) Gauge invariance links this stiffness to the mass of the photon field,

Table 16.1: **Parallels between Superconductivity and the Kondo effect .**

	Superconductivity	Kondo effect
Bound State	$\psi_\uparrow(x)\psi_\downarrow(x') = F(x-x')$ Bosonic	$(\vec{\sigma}_{\alpha\beta}\cdot\vec{S}(t'))\psi_\beta(t) = \Delta(t-t')f_\alpha(t')$ Fermionic
Characteristic energy Energy range contributing to bound state	$T_c = \omega_D e^{-1/g\rho}$ $E \in [T_c, \omega_D]$	$T_K = D\sqrt{J\rho}e^{-1/J\rho}$ $E \in [T_K, D]$
Extended in	space $\xi \sim v_F/T_c$	time $\tau \sim \hbar/T_K$
Conserved Quantity	Total electron charge	Charge of local moment
Long Range Order	LRO $d > 2$ Powerlaw in space $d \le 2$	Powerlaw in time
Phase stiffness	ρ_s	ρ_ϕ
Consequences of Phase stiffness (Anderson- Higgs) Quantity related to phase stiffness	Meissner effect $\frac{1}{\lambda_L^2} \propto \rho_s$	Formation of charged heavy electron $2\frac{\Delta V_c}{(2\pi)^3} = n_e + n_{spins}$ $\frac{1}{U^*} = \rho_\phi$

which generates the Meissner effect; the inverse squared penetration depth is directly proportional to the phase stiffness. In an analogous fashion, in the Kondo effect, the energy depends on temporal derivatives of the phase and the phase stiffness is [4]

$$E \propto \frac{\rho_\phi}{2}(\partial_t\phi)^2$$

For a Kondo lattice, there is one independent Kondo phase for each spin site, and the independent conservation of Q at each site guarantees that there is no spatial phase stiffness associated with ϕ. The temporal phase stiffness leads to a slow logarithmic growth in the phase -phase correlation functions, which in turn leads to power-law temporal correlations in the order parameter $V(\tau)$:

$$\langle\delta\phi(\tau)\delta\phi(\tau')\rangle \sim \frac{1}{N}\ln(\tau-\tau'), \qquad \langle\bar{V}(\tau)V(\tau')\rangle \sim e^{-\langle\delta\phi(\tau)\delta\phi(\tau')\rangle} \sim (\tau-\tau')^{-\frac{1}{N}}.$$

In this respect, the Kondo ground-state resembles a two dimensional superconductor, or a one dimensional metal: it is critical but has no true long-range order. As in the superconductor, the development of phase stiffness involves real physics. When we make a gauge transformation of the electromagnetic field,

$$\begin{aligned} e\Phi(x,t) &\to e\Phi(x,t) + \partial_t\alpha(x,t), \\ e\vec{A}(x,t) &\to e\vec{A}(x,t) + \nabla\alpha, \\ \psi(x) &\to \psi(x)e^{-i\alpha(x,t)} \end{aligned} \tag{16.42}$$

Because of the Anderson - Higg's effect, the hybridization is real and the only way to keep L_I invariant under the above transformation, is by gauge transforming the $f-$electron and the constraint field

$$\begin{aligned} f_\sigma(j) &\to f_\sigma(j)e^{-i\alpha(x_j,t)} \\ \lambda &\to \lambda + \partial_t\alpha \end{aligned} \tag{16.43}$$

(Notice how λ transforms in exactly the same way as the potential $e\Phi$.)

The non-trivial transformation of the $f-$electron under electromagnetic gauge transformations confirm that it has acquired a charge. Rigidity of the Kondo phase is thus intimately related to the formation of a composite charged fermion. The gauge invariant form for the energy dependence of the Kondo effect on the Kondo phase ϕ must then be

$$E \propto \frac{\rho_\phi}{2}(\partial_t\phi - e\Phi)^2$$

From the coefficient of Φ^2, we see that the Kondo cloud has an intrinsic capacitance $C = e^2\rho_\phi$ ($E \sim C\Phi^2/2$). But since the energy can also be written $(en_f)^2/2C \sim U^*n_f^2/2$ we see that the stiffness of the Kondo phase can also be associated with an interaction between the $f-$electrons of strength U^*, where

$$\frac{1}{U^*} = C/e^2 = \rho_\phi$$

[4]Note that because $\lambda \sim \partial_t\phi$, the phase stiffness is given by $\rho_\phi = \partial^2 F/\partial\lambda^2$

16.1.4 Mean-field theory of the Kondo Lattice

Diagonalization of the Hamiltonian

We can now make the bold jump from the single impurity problem, to the lattice. Most of the methods described in the last subsection generalize very naturally from the impurity to the lattice: the main difficulty is to understand the underlying physics. The mean-field Hamiltonian for the lattice[11**?**] takes the form

$$H_{MFT} = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + \sum_{j,\alpha} \left(f^\dagger{}_{j\alpha} \psi_{j\alpha} V_o + \bar{V}_o \psi^\dagger{}_{j\beta} f_{j\beta} + \lambda_o f^\dagger{}_{j\alpha} f_{j\alpha} \right) + Nn \left(\frac{\bar{V}_o V_o}{J} - \lambda_o q \right),$$

where n is the number of sites in the lattice. Notice, before we begin, that the composite f-state at each site of the lattice is entirely local, in that hybridization occurs at one site only. Were the composite f-state to be in any way non-local, we would expect that the hybridization of one f-state would involve conduction electrons at different sites. We begin by rewriting the mean field Hamiltonian in momentum space, as follows

$$H_{MFT} = \sum_{\vec{k}\sigma} \left(c^\dagger{}_{\vec{k}\sigma}, f^\dagger{}_{\vec{k}\sigma} \right) \begin{pmatrix} \epsilon_{\vec{k}} & V_o \\ V_o & \lambda_o \end{pmatrix} \begin{pmatrix} c_{\vec{k}\sigma} \\ f_{\vec{k}\sigma} \end{pmatrix} + Nn \left(\frac{\bar{V}_o V_o}{J} - \lambda_o q \right)$$

where

$$f^\dagger{}_{\vec{k}\sigma} = \frac{1}{\sqrt{n}} \sum_j f^\dagger{}_{j\sigma} e^{i\vec{k}\cdot\vec{R}_j}$$

is the Fourier transform of the $f-$electron field. The absence of $k-$ dependence in the hybridization is evident that each composite $f-$electron is spatially local. This Hamiltonian can be diagonalized in the form

$$H_{MFT} = \sum_{\vec{k}\sigma} \left(a^\dagger{}_{\vec{k}\sigma}, b^\dagger{}_{\vec{k}\sigma} \right) \begin{pmatrix} E_{\vec{k}+} & 0 \\ 0 & E_{\vec{k}-} \end{pmatrix} \begin{pmatrix} a_{\vec{k}\sigma} \\ b_{\vec{k}\sigma} \end{pmatrix} + Nn \left(\frac{\bar{V}_o V_o}{J} - \lambda_o q \right)$$

where $a^\dagger{}_{\vec{k}\sigma}$ and $b^\dagger{}_{\vec{k}\sigma}$ are linear combinations of $c^\dagger{}_{\vec{k}\sigma}$ and $f^\dagger{}_{\vec{k}\sigma}$, playing the role of "quasiparticle operators" of the theory and the momentum state eigenvalues $E_{\vec{k}\pm}$ of this Hamiltonian are determined by the condition

$$\mathrm{Det} \left[E_{\vec{k}\pm} 1 - \begin{pmatrix} \epsilon_{\vec{k}} & V_o \\ V_o & \lambda_o \end{pmatrix} \right] = 0,$$

which gives

$$E_{\vec{k}\pm} = \frac{\epsilon_{\vec{k}} + \lambda_o}{2} \pm \left[\left(\frac{\epsilon_{\vec{k}} - \lambda_o}{2} \right)^2 + |V_o|^2 \right]^{\frac{1}{2}} \tag{16.44}$$

are the energies of the upper and lower bands. The dispersion described by these energies is shown in Fig. 16.8 . A number of points can be made about this dispersion:

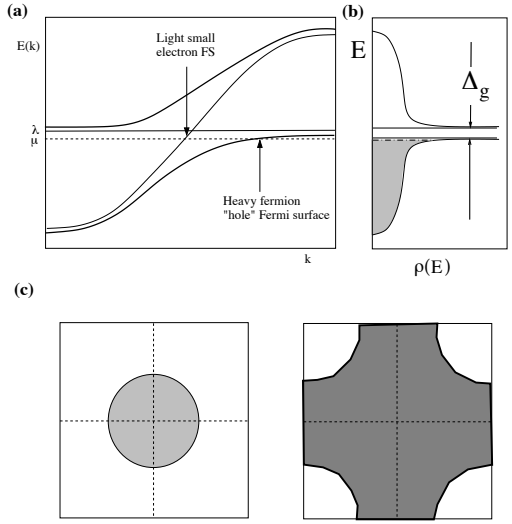


Figure 16.8: (a) Dispersion produced by the injection of a composite fermion into the conduction sea. (b) Renormalized density of states, showing "hybridization gap" (Δ_g). (c) Transformation of the Fermi surface from a light electron Fermi surface into a heavy "hole"-like Fermi surface.

- We see that the Kondo effect injects new fermionic states into the the original conduction band. Hybridization between the heavy electron states and the conduction electrons builds an upper and lower Fermi band separated by a "hybridization gap" of width $\Delta_g = E_g(+) - E_g(-)$, such that energies in the range

$$\begin{aligned} E_g(-) < \quad E \quad &< \lambda_o + E_g(+) \\ E_g(\pm) \quad = \quad \lambda_o &\pm \frac{V_0^2}{D_\mp} \end{aligned} \tag{16.45}$$

  are forbidden. Here $\pm D_\pm$ are the top and bottom of the conduction band. In the special case where $\lambda_o = 0$, corresponding to half filling, a Kondo insulator is formed.

- The effective mass of the Fermi surface has the opposite sign to the original conduction sea from which it is built, so naively, the Hall constant should change sign when coherence develops.

- The Fermi surface volume expands in response to the presence of the new heavy electron

bands. The new Fermi surface volume now counts the total number of particles. To see this note that

$$N_{tot} = \langle \sum_{k\lambda\sigma} n_{k\lambda\sigma} \rangle = \langle \hat{n}_f + n_c \rangle$$

where $n_{k\lambda\sigma} = a^\dagger_{k\lambda\sigma} a_{k\lambda\sigma}$ is the number operator for the quasiparticles and n_c is the total number of conduction electrons. This means

$$N_{tot} = N\frac{V_{FS}}{(2\pi)^3} = Q + n_c.$$

This expansion of the Fermi surface is a direct manifestation of the creation of new states by the Kondo effect. It is perhaps worth stressing that these new states would form, even if the local moments were nuc In other words, they are electronic states that have only depend on the rotational degrees of freedom of the local moments.

The Free energy of this system is then

$$\frac{F}{N} = -T\sum_{\vec{k},\pm} \ln\left[1 + e^{-\beta E_{\vec{k}\pm}}\right] + n_s\left(\frac{\bar{V}V}{J} - \lambda q\right)$$

Let us discuss the ground-state energy, E_o- the limiting $T \to 0$ of this expression. We can write this in the form

$$\frac{E_o}{Nn_s} = \int_{-\infty}^{0} \rho^*(E)E + \left(\frac{\bar{V}V}{J} - \lambda q\right)$$

where we have introduced the density of heavy electron states $\rho^*(E) = \sum_{\vec{k},\pm} \delta(E - E^{(\pm)}_{\vec{k}})$. Now the relationship between the energy of the heavy electrons (E) and the energy of the conduction electrons (ϵ) is given by

$$E = \epsilon + \frac{V^2}{E - \lambda}$$

so that the density of heavy electron states related to the conduction electron density of states ρ by

$$\rho^*(E) = \rho\frac{d\epsilon}{dE} = \rho\left(1 + \frac{V^2}{(E-\lambda)^2}\right) \tag{16.46}$$

The originally flat conduction electron density of states is now replaced by a "hybridization gap", flanked by two sharp peaks of width approximately $\pi\rho V^2 \sim T_K$. With this information, we can carry out the integral over the energies, to obtain

$$\frac{E_o}{Nn_s} = \frac{D^2\rho}{2} + \int_{-D}^{0} d\epsilon\rho\bar{V}V\frac{E}{(E-\lambda)^2} + \left(\frac{\bar{V}V}{J} - \lambda q\right) \tag{16.47}$$

where we have assumed that the upper band is empty, and the lower band is partially filled. If we impose the constraint $\frac{\partial F}{\partial \lambda} = \langle n_f \rangle - Q = 0$ we obtain

$$\frac{\Delta}{\pi\lambda} - q = 0$$

so that the ground-state energy can be written

$$\frac{E_o}{Nn_s} = \frac{\Delta}{\pi}\ln\left(\frac{\Delta e}{\pi q T_K}\right) \tag{16.48}$$

where $T_K = De^{-\frac{1}{J\rho}}$ as before.

Let us pause for a moment to consider this energy functional qualitatively. The Free energy surface has the form of "Mexican Hat" at low temperatures. The minimum of this functional will then determine a familiy of saddle point values $V = V_o e^{i\theta}$, where θ can have any value. If we differentiate the ground-state energy with respect to V^2, we obtain

$$0 = \frac{1}{\pi}\ln\left(\frac{\Delta e^2}{\pi q T_K}\right)$$

or

$$\Delta = \frac{\pi q}{e^2}T_K$$

confirming that $\Delta \sim T_K$.

Composite Nature of the heavy quasiparticle in the Kondo lattice.

We now turn to discuss the nature of the heavy quasiparticles in the Kondo lattice. Clearly, at an operational level, the composite $f-$electrons are formed in the same way as in the impurity model, but at each site, i.e

$$\frac{1}{N}\Gamma_{\alpha\beta}(j,t)\psi_{j\alpha}(t) \to \left(\frac{\bar{V}}{J}\right)f_{j\alpha}(t)$$

This composite object admixes with conduction electrons at a single site- site j. The bound-state amplitude in this expression can be written

$$-\frac{V_o}{J} = \frac{1}{N}\langle f^\dagger_\beta \psi_\beta \rangle \tag{16.49}$$

To evaluate the contributions to this sum, it is useful to notice that the condition $\partial E/\partial\bar{V} = 0$ can be written

$$\begin{aligned}\frac{1}{N}\frac{\partial E}{\partial \bar{V}_o} &= 0 = \frac{V_o}{J} + \frac{1}{N}\langle f^\dagger_\beta\psi_\beta\rangle \\ &= \frac{V_o}{J} + V_o\int_{-D}^{0} d\epsilon\rho\frac{E}{(E-\lambda)^2}\end{aligned} \tag{16.50}$$

where we have used (16.47) to evaluate the derivative. From this we see that we can write

$$\begin{aligned}\frac{V_o}{J} &= -V_o\int_{-D}^{0} d\epsilon\rho\left(\frac{1}{E-\lambda} + \frac{\lambda}{(E-\lambda)^2}\right) \\ &= -V_o\rho\ln\left[\frac{\lambda e}{D}\right]\end{aligned} \tag{16.51}$$

It is clear that as in the impurity, the composite $f-$electrons in the Kondo lattice are formed from *high energy* electron states all the way out to the bandwidth. In a similar fashion to the impurity, each decade of energy between T_K and D contributes equally to the overall bound-state amplitude. The above expression only differs from the corresponding impurity expression (16.36) at low energies, showing that low energy electrons play a comparatively unimportant role in forming the composite heavy electron. It is this feature that permits a dense array of composite fermions to co-exist throughout the crystal lattice.

These composite $f-$electrons admix with the conduction electrons to produce a heavy electron band with a density of states given by (16.46),

$$\rho^*(E) = \rho\frac{d\epsilon}{dE} = \rho\left(1 + \frac{V^2}{(E-\lambda)^2}\right)$$

which becomes

$$\rho^*(0) = \rho + \frac{q}{T_K}$$

at the Fermi energy. The mass enhancement of the heavy electrons is then

$$\frac{m^*}{m} = 1 + \frac{q}{\rho T_K} \sim \frac{qD}{T_K}$$

This large factor in the effective mass enhancement can be as much as 1000 in the most severely renormalized heavy electron systems.

Consequences of mass renormalization

The effective mass enhancement of heavy electrons can be directly observed in a wide range of experimental quantities including

- The large renormalization of the linear specific heat coefficient $\gamma^* \sim \frac{m^*}{m}\gamma$ and Pauli susceptibility $\chi^* \sim \frac{m^*}{m}\chi$.
- The quadratic temperature (" A") coefficient of the resistivity. At low temperatures the resistivity of a Fermi liquid has a quadratic temperature dependence, $\rho \sim \rho_o + AT^2$, where $A \sim \left(\frac{1}{T_F}\right)^2 \sim \left(\frac{m^*}{m}\right)^2 \sim \gamma^2$ is related to the density of three-particle excitations. The approximate constancy of the ratio A/γ^2 in heavy fermion systems is known as the "Kadowaki-Woods" relation.[12]
- The renormalization of the effective mass as measured by dHvA measurements of heavy electron Fermi surfaces.[**? ? ?**]
- The appearance of a heavy quasiparticle Drude feature in the frequency dependent optical conductivity $\sigma(\omega)$. (See discussion below).

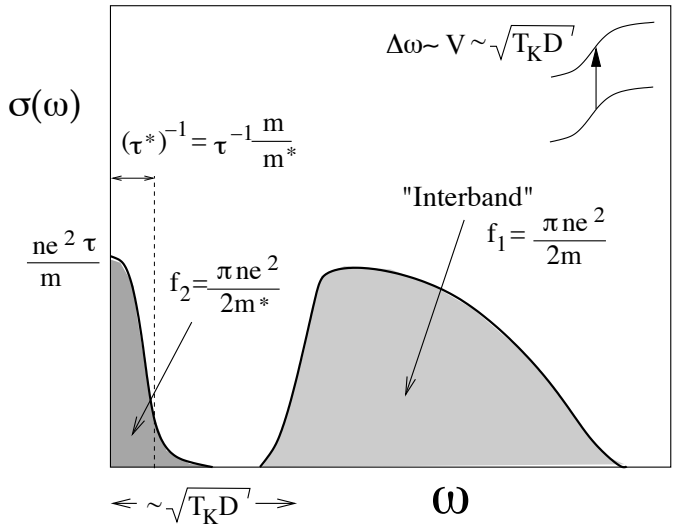


Figure 16.9: Separation of the optical sum rule in a heavy fermion system into a high energy "interband" component of weight $f_2 \sim ne^2/m$ and a low energy Drude peak of weight $f_1 \sim ne^2/m^*$.

The optical conductivity of heavy fermion metals deserves special discussion. According to the f-sum rule, the total integrated optical conductivity is determined by the plasma frequency

$$\int_0^\infty \frac{d\omega}{\pi}\sigma(\omega) = f_1 = \frac{\pi}{2}\left(\frac{ne^2}{m}\right)$$

where n is the density of electrons. [5] In the absence of local moments, this is the total spectral weight inside the Drude peak of the optical conductivity.

[5]The f-sum rule is a statement about the instantaneous, or short-time diamagnetic response of the metal. At short times $dj/dt = (ne^2/m)E$, so the high frequency limit of the conductivity is $\sigma(\omega) = \frac{ne^2}{m}\frac{1}{\delta - i\omega}$. But using the Kramer's Krönig relation

$$\sigma(\omega) = \int \frac{dx}{i\pi}\frac{\sigma(x)}{x - \omega - i\delta}$$

at large frequencies,

$$\omega(\omega) = \frac{1}{\delta - i\omega}\int \frac{dx}{\pi}\sigma(x)$$

so that the short-time diamagnetic response implies the f-sum rule.

What happens to this spectral weight when the heavy electron fluid forms? Whilst we expect this sum rule to be preserved, we also expect a new "quasiparticle" Drude peak to form in which

$$\int d\omega\sigma(\omega) = f_2\frac{\pi}{2}\frac{ne^2}{m^*} = f_1\frac{m}{m^*}$$

In other words, we expect the total spectral weight to divide up into a tiny "heavy fermion" Drude peak, of total weight f_2, where

$$\sigma(\omega) = \frac{ne^2}{m^*}\frac{1}{(\tau^*)^{-1} - i\omega}$$

separated off by an energy of order $V \sim \sqrt{T_K D}$ from an "inter-band" component associated with excitations between the lower and upper Kondo bands.[13, 14] This second term carries the bulk $\sim f_1$ of the spectral weight. (Fig. 16.9).

Simple calculations, based on the Kubo formula confirm this basic expectation,[13, 14] showing that the relationship between the original relaxation rate of the conduction sea and the heavy electron relaxation rate τ^* is

$$(\tau^*)^{-1} = \frac{m}{m^*}(\tau)^{-1}. \tag{16.52}$$

Notice that this means that the residual resistivity

$$\rho_o = \frac{m^*}{ne^2\tau^*} = \frac{m}{ne^2\tau}$$

is unaffected by the effects of mass renormalization. This can be understood by observing that the heavy electron Fermi velocity is also renormalized by the effective mass, $v_F^* = \frac{m}{m^*}$, so that the mean-free path of the heavy electron quasiparticles is unaffected by the Kondo effect.

$$l^* = v_F^*\tau^* = v_F\tau$$

This is yet one more reminder that the Kondo effect is local in space, yet non-local in time.

These basic features- the formation of a narrow Drude peak, and the presence of a hybridization gap, have been seen in optical measurements on heavy electron systems[**?** 15**?**]

16.1.5 Summary

In this lecture we have presented Doniach's argument that the enhancement of the Kondo temperature over and above the characteristic RKKY magnetic interaction energy between spins leads to the formation of a heavy electron ground-state. This enhancement is thought to be generated by the large spin degeneracies of rare earth, or actinide ions. A simple mean-field theory of the Kondo model and Kondo lattice, which ignores the RKKY interactions, provides a unified picture of heavy electron formation and the Kondo effect, in terms of the formation of a composite quasiparticle between high energy conduction band electrons and local moments. This basic physical effect is local in space, but non-local in time. Certain analogies can be struck between Cooper pair formation, and the formation of the heavy electron bound-state, in particular, the charge on the $f-$electron can be seen as a direct consequence of the temporal phase stiffness of the Kondo bound-state. This bound-state hybridizes with conduction electrons- producing a single isolated resonance in a Kondo impurity, and an entire renormalized Fermi surface in the Kondo lattice.

16.2 Exercises

1. (a) Using the identity $n_{f\sigma}^2 = n_{f\sigma}$, show that the atomic part of the Anderson model can be written in the form

$$H_{atomic} = (E_f + \frac{U}{2})n_f + \frac{U}{2}\Big[(n_f - 1)^2 - 1\Big], \tag{16.53}$$

What happens when $E_f + U/2 = 0$?

(b) Using the completeness relation

$$\overbrace{|f^0\rangle\langle f^0| + |f^2\rangle\langle f^2|}^{(n_f-1)^2} + \overbrace{|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|}^{\mathbf{S}^2}\frac{}{S(S+1)} = 1. \qquad (S = 1/2)$$

show that the interaction can also be written in the form

$$H_{atomic} = (E_f + \frac{U}{2})n_f - \frac{2U}{3}\mathbf{S}^2 \tag{16.54}$$

which makes it clear that the repulsive U term induces a "magnetic attraction" that favors formation of a local moment.

(c) Derive the Hubbard Stratonovich decoupling for (16.54).

2. By expanding a plane wave state in terms of spherical harmonics:

$$\langle\mathbf{r}|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi\sum_{l,m} i^l j_l(kr)Y_{lm}^*(\hat{\mathbf{k}})Y_{lm}(\hat{\mathbf{r}})$$

show that the overlap between a state $|\psi\rangle$ with wavefunction $\langle\vec{x}|\psi\rangle = R(r)Y_{lm}(\hat{r})$ with a plane wave is given by $V(\vec{k}) = \langle\vec{k}|V|\psi\rangle = V(k)Y_{lm}(\hat{k})$ where

$$V(k) = 4\pi i^{-l}\int dr r^2 V(r)R(r)j_l(kr) \tag{16.55}$$

3. (i) Show that $\delta = \cot^{-1}\left(\frac{E_d}{\Delta}\right)$ is the scattering phase shift for scattering off a resonant level at position E_d.

   (ii) Show that the energy of states in the continuum is shifted by an amount $-\Delta\epsilon\delta(\epsilon)/\pi$, where $\Delta\epsilon$ is the separation of states in the continuum.

   (iii) Show that the increase in density of states is given by $\partial\delta/\partial E = \rho_d(E)$. (See chapter 3.)

4. Generalize the scaling equations to the anisotropic Kondo model with an anisotropic interaction

$$H_I = \sum_{|\epsilon_k|,|\epsilon_{k'}|,a=(x,y,z)} J^a c^\dagger{}_{k\alpha}\sigma^a_{\alpha\beta}c_{k'\beta}\cdot S^a{}_d \tag{16.56}$$

and show that the scaling equations take the form

$$\frac{\partial J_a}{\partial\ln D} = -2J_bJ_c\rho + O(J^3),$$

where and (a, b, c) are a cyclic permutation of (x, y, z). Show that in the special case where $J_x = J_y = J_\perp$, the scaling equations become

$$\begin{aligned}\frac{\partial J_\perp}{\partial \ln D} &= -2J_z J_\perp \rho + O(J^3),\\ \frac{\partial J_z}{\partial \ln D} &= -2(J_z)^2\rho + O(J^3),\end{aligned} \tag{16.57}$$

so that $J_z^2 - J_\perp^2 =$ constant. Draw the corresponding scaling diagram.

5. Consider the symmetric Anderson model, with a symmetric band-structure at half filling. In this model, the d^0 and d^2 states are degenerate and there is the possibility of a "charged Kondo effect" when the interaction U is negative. Show that under the "particle-hole" transformation

$$\begin{aligned} c_{k\uparrow} &\to c_{k\uparrow}, \qquad d_\uparrow \to d_\uparrow\\ c_{k\downarrow} &\to -c^\dagger_{k\downarrow}, \qquad d_\downarrow \to -d^\dagger_\downarrow\end{aligned} \tag{16.58}$$

the positive U model is transformed to the negative U model. Show that the spin operators of the local moment are transformed into Nambu "isospin operators" which describe the charge and pair degrees of freedom of the d-state. Use this transformation to argue that when U is negative, a charged Kondo effect will occur at exactly half-filling involving quantum fluctuations between the degenerate d^0 and d^2 configurations.

6. What happens to the Schrieffer-Wolff transformation in the infinite U limit? Rederive the Schrieffer-Wolff transformation for an N-fold degenerate version of the infinite U Anderson model. This is actually valid for Ce and Yb ions.

7. Rederive the Nozières Fermi liquid picture for an SU (N) degenerate Kondo model. Explain why this picture is relevant for magnetic rare earth ions such as Ce^{3+} or Yb^{3+}.

8. Check the Popov trick works for a magnetic moment in an external field. Derive the partition function for a spin in a magnetic field using this method.

9. Use the Popov trick to calculate the T-matrix diagrams for the leading Kondo renormalization diagramatically.

10. Derive the formula (15.66) for the conductance of a single isolated resonance.

11. (a) Directly confirm the Read-Newn's gauge transformation (16.41).

    (b) Directly calculate the "phase stiffness" $\rho_\phi = -\frac{d^2F}{d\lambda^2}$ of the large N Kondo model and show that at $T = 0$.

$$\rho_\phi = \frac{N}{\pi}\left(\frac{\sin(\pi q)}{T_K}\right).$$

12. (a) Introduce a simple relaxation time into the conduction electron propagator, writing

$$G(\vec{k}, i\omega_n)^{-1} = i\omega_n + i\mathrm{sgn}(\omega_n)/2\tau + \frac{V^2}{i\omega_n - \lambda} \tag{16.59}$$

Show that the poles of this Greens function occur at

$$\omega = E_k \pm \frac{i}{2\tau^*}$$

where

$$\tau^* = \frac{m^*}{m}\tau$$

is the renormalized elestic scattering time.

(b) The Kubo formula for the optical conductivity of an isotropic one-band system is

$$\sigma(\nu) = -\frac{Ne^2}{3}\sum_k v_k^2 \frac{\Pi(\nu)}{i\nu}$$

where we have used the N fold spin degeneracy, and $\Pi(\nu)$ is the analytic extension of

$$\Pi(i\nu_n) = T\sum_m G(\vec{k}, i\omega_m)\left[G(\vec{k}, i\omega_m + i\nu_n) - G(\vec{k}, i\omega_m)\right]$$

where in our case, $G(\vec{k}, i\omega_n)$ is the conduction electron propagator. Using (16.59), and approximating the momentum sum by an integral over energy, show that the low frequency conductivity of the large N Kondo lattice is given by

$$\sigma(\nu) = \frac{ne^2}{m^*}\frac{1}{(\tau^*)^{-1} - i\nu}.$$

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