

The Heisenberg representation removes all time-dependence from the wavefunction, so that $|\psi_H\rangle = |\psi_s(0)\rangle$ and all time-evolution is transferred to the operators,

$$A_H(\tau) = e^{iH(-i\tau)} A_S e^{-iH(-i\tau)} = e^{H\tau} A_S e^{-H\tau}. \quad (9.6)$$

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

$$H = \sum \epsilon_k c_k^\dagger c_k$$

we obtain

$$\begin{aligned} \frac{\partial c_k}{\partial \tau} &= [H, c_k] = -\epsilon_k c_k \\ \frac{\partial c_k^\dagger}{\partial \tau} &= [H, c_k^\dagger] = \epsilon_k c_k^\dagger \end{aligned} \quad (9.7)$$

so that

$$\left. \begin{aligned} c_k(\tau) &= e^{-\epsilon_k \tau} c_k \\ c_k^\dagger(\tau) &= e^{\epsilon_k \tau} c_k^\dagger \end{aligned} \right\} \quad (\text{p.s.} \quad c_k^\dagger(\tau) = (c_k(-\tau))^\dagger \neq (c_k(\tau))^\dagger). \quad (9.8)$$

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

$$\begin{aligned} -\frac{\partial}{\partial \tau} U(\tau) &= -\frac{\partial}{\partial \tau} [e^{H_0\tau} e^{-H\tau}] \\ &= e^{H_0\tau} V e^{-H\tau} \\ &= e^{H_0\tau} V e^{-H_0\tau} U(\tau) \\ &= V_I(\tau) U(\tau) \end{aligned} \quad (9.9)$$

and a similar equation applies to $S(\tau_1, \tau_2)$,

$$-\frac{\partial}{\partial \tau} S(\tau_1, \tau_2) = V_I(\tau) S(\tau_1, \tau_2). \quad (9.10)$$

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

$$\begin{aligned} U(\tau) &= T \exp \left[-\int_0^\tau V_I(\tau) d\tau \right] \\ S(\tau_1, \tau_2) &= T \exp \left[-\int_{\tau_1}^{\tau_2} V_I(\tau) d\tau \right]. \end{aligned} \quad (9.11)$$

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

$$\begin{aligned} Z &= \text{Tr} [e^{-\beta H}] = \text{Tr} [e^{-\beta H_0} U(\beta)] \\ &= \frac{Z_0}{\text{Tr} [e^{-\beta H_0}]} \left(\frac{\text{Tr} [e^{-\beta H_0} U(\beta)]}{\text{Tr} [e^{-\beta H_0}]} \right) \\ &= Z_0 \langle U(\beta) \rangle_0 \end{aligned} \quad (9.12)$$

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.

$$\frac{Z}{Z_0} = e^{-\beta \Delta F} = \langle T \exp \left[-\int_0^\beta V_I(\tau) d\tau \right] \rangle \quad (9.13)$$

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

$$\mathcal{G}_{\lambda\lambda'}(\tau - \tau') = -\langle T \psi_\lambda(\tau) \psi_{\lambda'}^\dagger(\tau') \rangle = -T r [e^{-\beta(H-F)} \psi_\lambda(\tau) \psi_{\lambda'}^\dagger(\tau')] \quad (9.14)$$

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

$$H = \sum \epsilon_\lambda \psi_\lambda^\dagger \psi_\lambda, \quad (9.15)$$

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

$$\langle \psi_{\lambda'}^\dagger \psi_\lambda \rangle = \delta_{\lambda\lambda'} \begin{cases} n(\epsilon_\lambda) & \text{(Bosons)} \\ f(\epsilon_\lambda) & \text{(Fermions)} \end{cases} \quad (9.16)$$

where

$$\begin{aligned} n(\epsilon_\lambda) &= \frac{1}{e^{\beta\epsilon_\lambda} - 1} \\ f(\epsilon_\lambda) &= \frac{1}{e^{\beta\epsilon_\lambda} + 1} \end{aligned} \quad (9.17)$$

are the Bose and Fermi functions respectively. Similarly,

$$\langle \psi_\lambda \psi_{\lambda'}^\dagger \rangle = \delta_{\lambda\lambda'} \pm \langle \psi_{\lambda'}^\dagger \psi_\lambda \rangle = \delta_{\lambda\lambda'} \begin{cases} 1 + n(\epsilon_\lambda) & \text{(Bosons)} \\ 1 - f(\epsilon_\lambda) & \text{(Fermions)} \end{cases} \quad (9.18)$$

Using the time evolution of the operators,

$$\begin{aligned} \psi_\lambda(\tau) &= e^{-\epsilon_\lambda \tau} \psi_\lambda(0) \\ \psi_\lambda^\dagger(\tau) &= e^{\epsilon_\lambda \tau} \psi_\lambda^\dagger(0) \end{aligned} \quad (9.19)$$

we deduce that

$$\mathcal{G}_{\lambda\lambda'}(\tau - \tau') = - \left[\theta(\tau - \tau') \langle \psi_\lambda \psi_{\lambda'}^\dagger \rangle + \zeta \theta(\tau' - \tau) \langle \psi_{\lambda'}^\dagger \psi_\lambda \rangle \right] e^{-\epsilon_\lambda(\tau - \tau')} \quad (9.20)$$

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

$$\mathcal{G}_\lambda(\tau) = -e^{-\epsilon_\lambda \tau} \begin{cases} [(1 + n(\epsilon_\lambda))\theta(\tau) + n(\epsilon_\lambda)\theta(-\tau)] & \text{(Bosons)} \\ [(1 - f(\epsilon_\lambda))\theta(\tau) - f(\epsilon_\lambda)\theta(-\tau)] & \text{(Fermions)} \end{cases} \quad (9.21)$$

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

$$\begin{aligned} \mathcal{G}_{\lambda\lambda'}(\tau) &= \zeta \langle \psi_{\lambda'}^\dagger(0) \psi_\lambda(\tau) \rangle \\ &= \zeta \text{Tr} \left[e^{-\beta(H-F)} \psi_{\lambda'}^\dagger e^{\tau H} \psi_\lambda e^{-\tau H} \right] \end{aligned} \quad (9.22)$$

Now we can use the periodicity of the trace $\text{Tr}(AB) = \text{Tr}(BA)$ to cycle the operators on the left of the trace over to the right of the trace, as follows

$$\begin{aligned} \mathcal{G}_{\lambda\lambda'}(\tau) &= \zeta \text{Tr} \left[e^{\tau H} \psi_\lambda e^{-\tau H} e^{-\beta(H-F)} \psi_{\lambda'}^\dagger \right] \\ &= \zeta \text{Tr} \left[e^{\beta F} e^{\tau H} \psi_\lambda e^{-(\tau+\beta)H} \psi_{\lambda'}^\dagger \right] \\ &= \zeta \text{Tr} \left[e^{-\beta(H-F)} e^{(\tau+\beta)H} \psi_\lambda e^{-(\tau+\beta)H} \psi_{\lambda'}^\dagger \right] \\ &= \zeta \text{Tr} \langle \psi_\lambda(\tau + \beta) \psi_{\lambda'}^\dagger(0) \rangle \\ &= \zeta \mathcal{G}_{\lambda\lambda'}(\tau + \beta) \end{aligned} \quad (9.23)$$

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

$$\begin{aligned} \nu_n &= 2\pi n k_B T & \text{(Boson)} \\ \omega_n &= \pi(2n + 1) k_B T & \text{(Fermion)}. \end{aligned} \quad (9.24)$$

where by convention, ν_n is reserved for Bosons and ω_n for fermions. These frequencies have the property that

$$\begin{aligned} e^{i\nu_n(\tau+\beta)} &= e^{i\nu_n\tau} \\ e^{i\omega_n(\tau+\beta)} &= -e^{i\omega_n\tau} \end{aligned} \quad (9.25)$$

The periodicity or antiperiodicity of the Green function is then captured by expanding it as a linear sum of these functions:

$$\mathcal{G}_{\lambda\lambda'}(\tau) = \begin{cases} T \sum_n \mathcal{G}_{\lambda\lambda'}(i\nu_n) e^{-i\nu_n\tau} & \text{Boson} \\ T \sum_n \mathcal{G}_{\lambda\lambda'}(i\omega_n) e^{-i\omega_n\tau} & \text{Fermion} \end{cases} \quad (9.26)$$

and the inverse of these relations is given by

$$\mathcal{G}_{\lambda\lambda'}(i\alpha_n) = \int_0^\beta d\tau \mathcal{G}_{\lambda\lambda'}(\tau) e^{i\alpha_n\tau}, \quad (\alpha_n = \{\text{Matsubara frequency}\}) \quad (9.27)$$

Example : Free Fermions and Free Bosons

For example, let us use (9.27) to derive the propagator for non-interacting fermions or bosons with $H = \sum \epsilon_\lambda \psi_\lambda^\dagger \psi_\lambda$. For fermions, the Matsubara frequencies are $i\omega_n = \pi(2n+1)k_B T$ so using the real time propagator(9.21), we obtain

$$\begin{aligned} \mathcal{G}_\lambda(i\omega_n) &= - \int_0^\beta d\tau e^{(i\omega_n - \epsilon_\lambda)\tau} \overbrace{(1 - f(\epsilon_\lambda))}^{[1 + e^{-\beta\epsilon_\lambda}]^{-1}} \\ &= - \frac{1}{i\omega_n - \epsilon_\lambda} \overbrace{(e^{(i\omega_n - \epsilon_\lambda)} - 1)}^{-1} \frac{1}{1 + e^{-\beta\epsilon_\lambda}} \end{aligned} \quad (9.28)$$

so that

$$\mathcal{G}_\lambda(i\omega_n) = \frac{1}{i\omega_n - \epsilon_\lambda} \quad \text{Free Fermions} \quad (9.29)$$

In a similar way, for free Bosons, where the Matsubara frequencies are $i\nu_n = \pi 2nk_B T$, using (9.27) and (9.21), we obtain

$$\begin{aligned} \mathcal{G}_\lambda(i\nu_n) &= - \int_0^\beta d\tau e^{(i\nu_n - \epsilon_\lambda)\tau} \overbrace{(1 + n(\epsilon_\lambda))}^{[1 - e^{-\beta\epsilon_\lambda}]^{-1}} \\ &= - \frac{1}{i\nu_n - \epsilon_\lambda} \overbrace{(e^{(i\nu_n - \epsilon_\lambda)} - 1)}^{-1} \frac{1}{1 - e^{-\beta\epsilon_\lambda}} \end{aligned} \quad (9.30)$$

so that

$$\mathcal{G}_\lambda(i\nu_n) = \frac{1}{i\nu_n - \epsilon_\lambda} \quad \text{Free Bosons} \quad (9.31)$$

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 $\omega \rightarrow i\omega_n$ 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

$$D(\tau) = -\langle T x(\tau)x(0) \rangle \quad (9.32)$$

and its corresponding propagator

$$D(i\nu) = \int_0^\beta e^{i\nu\tau} D(\tau) \quad (9.33)$$

for the simple harmonic oscillator

$$\begin{aligned} H &= \hbar\omega(b^\dagger b + \frac{1}{2}) \\ x &= \sqrt{\frac{\hbar}{2m\omega}}(b + b^\dagger) \end{aligned} \quad (9.34)$$

Expanding the Green function in terms of the creation and annihilation operators, we have

$$\begin{aligned} D(\tau) &= -\frac{\hbar}{2m\omega} \langle T(b(\tau) + b^\dagger(\tau))(b(0) + b^\dagger(0)) \rangle \\ &= -\frac{\hbar}{2m\omega} (\langle T b(\tau)b^\dagger(0) \rangle + \langle T b^\dagger(\tau)b(0) \rangle), \end{aligned} \quad (9.35)$$

where terms involving two creation or two annihilation operators vanish. Now using the derivations that led to (9.21)

$$-\langle T b(\tau)b^\dagger(0) \rangle = \mathcal{G}(\tau) = -(1 + n(\omega))\theta(\tau) + n(\omega)\theta(-\tau)e^{-\omega\tau}. \quad (9.36)$$

and

$$\begin{aligned} -\langle T b^\dagger(\tau)b(0) \rangle &= -[n(\omega)\theta(\tau) + (1 + n(\omega))]e^{\omega\tau} \\ &= [(1 + n(-\omega))\theta(\tau) + n(-\omega)\theta(-\tau)]e^{\omega\tau}. \end{aligned} \quad (9.37)$$

which corresponds to $-\mathcal{G}(\tau)$ with the sign of ω inverted. With this observation,

$$D(\tau) = \frac{\hbar}{2m\omega} [G(\tau) - \{\omega \rightarrow -\omega\}]. \quad (9.38)$$

When we Fourier transform the first term inside the brackets, we obtain $\frac{1}{i\nu_n - \omega}$, so that

$$\begin{aligned} D(i\nu_n) &= \frac{\hbar}{2m\omega} \left[\frac{1}{i\nu_n - \omega} - \frac{1}{i\nu_n + \omega} \right] \\ &= \frac{\hbar}{2m\omega} \left[\frac{2\omega}{(i\nu_n)^2 - \omega^2} \right]. \end{aligned} \quad (9.39)$$

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 $H = \sum_{\lambda} \epsilon_{\lambda} c_{\lambda}^{\dagger} c_{\lambda}$ 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

$$N(\mu) = T \sum_{\lambda} \mathcal{G}_{\lambda}(i\omega_n) e^{i\omega_n 0^+}$$

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

$$F(T, \mu) = -k_B T \sum_{\lambda, i\omega_n} \ln \left[-\mathcal{G}_{\lambda}(i\omega_n)^{-1} \right] e^{i\omega_n 0^+} + C(T) \quad (9.40)$$

Solution: The number of particles in state λ can be related to the equal time Green's function as follows

$$N_{\lambda} = \langle c_{\lambda}^{\dagger} c_{\lambda} \rangle = -\langle T c_{\lambda}(0^-) c_{\lambda}^{\dagger} \rangle = \mathcal{G}_{\lambda}(0^-).$$

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

$$\begin{aligned} F &= - \int^{\mu} d\mu N(\mu) = -T \sum_{\lambda, i\omega_n} \int^{\mu} d\mu \frac{e^{i\omega_n 0^+}}{i\omega_n - E_{\lambda} + \mu} \\ &= -T \sum_{\lambda, i\omega_n} \ln [\epsilon_{\lambda} - i\omega_n] e^{i\omega_n 0^+} \\ &= -T \sum_{\lambda, i\omega_n} \ln \left[-\mathcal{G}_{\lambda}(i\omega_n)^{-1} \right] e^{i\omega_n 0^+} + C(T). \end{aligned} \quad (9.41)$$

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

$$M = \mu_B \sum_{\lambda, \sigma} \sigma \langle c_{\lambda\sigma}^{\dagger} c_{\lambda\sigma} \rangle = \mu_B T \sum_{\mathbf{k}, \sigma, i\omega_n} \sigma \mathcal{G}_{\sigma}(\mathbf{k}, i\omega_n) e^{i\omega_n 0^+}$$

Differentiating this w.r.t. B and then setting $B = 0$, we obtain

$$\begin{aligned} \chi &= \left. \frac{\partial M}{\partial B} \right|_{B=0} = -\mu_B^2 T \sum_{\mathbf{k}, \sigma, i\omega_n} \sigma^2 \mathcal{G}_{\sigma}(\mathbf{k}, i\omega_n)^2 \Big|_{B=0} \\ &= -2\mu_B^2 k_B T \sum_{\mathbf{k}, i\omega_n} G(k)^2 \end{aligned} \quad (9.42)$$

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

$$\langle c_{\mathbf{p}\sigma}^{\dagger} c_{\mathbf{p}\sigma} \rangle = \mathcal{G}(\mathbf{p}, 0^-) = T \sum_n \frac{1}{i\omega_n - \epsilon(\mathbf{p})} e^{i\omega_n 0^+}. \quad (9.43)$$

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

$$\chi(q) = -2\mu_B^2 T \sum_p \mathcal{G}(p+q) \mathcal{G}(p) = 2\mu_B^2 \sum_p \left(k_B T \sum_r G(\mathbf{p} + \mathbf{q}, i\omega_r + i\nu_n) G(\mathbf{p}, i\omega_r) \right). \quad (9.44)$$

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

$$k_B T \sum_n F(i\omega_n) = - \int_C \frac{dz}{2\pi i} F(z) f(z) \quad (9.45)$$

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)

Our result for the electron propagator, ignoring the “vertex corrections” to the scattering self-energy is given by

$$G(\mathbf{k}, z) = \frac{1}{z - \epsilon_{\mathbf{k}} + i\frac{1}{2\tau} \text{sgnIm}(z)}$$

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”,

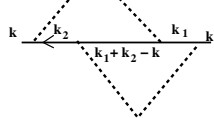
$$A(\mathbf{k}, \omega) = \frac{1}{\pi} \text{Im}G(\mathbf{k}, \omega - i\delta) = \frac{1}{\pi} \frac{(2\tau)^{-1}}{(\omega - \epsilon_{\mathbf{k}})^2 + (2\tau)^{-2}}$$

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

$$\Sigma_2 = N(0) \int \frac{d\epsilon_1}{i\omega_n - \epsilon_1} \overbrace{N(0) \int \frac{d\epsilon_2}{i\omega_n - \epsilon_2}}^{-i\frac{1}{2\tau}} \overbrace{\int \frac{d\Omega_1 d\Omega_2}{(4\pi)^2} \frac{1}{i\omega_n - \epsilon_{\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}}}}^{\sim \frac{1}{k_F v_F}}$$

$$\sim i\frac{1}{\tau} \times \frac{1}{k_F l} \tag{9.94}$$

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

$$\frac{\omega_D^2}{\epsilon_F^2} \sim \frac{1}{(\epsilon_F a^2)} \frac{1}{M} \sim \frac{m}{\sim 1/m}$$

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 continuously 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 $\omega_{q,\lambda}$. For the moment, we shall also ignore the Coulomb interaction between electrons. The Fröhlich Hamiltonian is then

$$\begin{aligned} H_e &= \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \\ H_p &= \sum_{\mathbf{q},\lambda} \omega_{q,\lambda} \left(a_{\mathbf{q},\lambda}^\dagger a_{\mathbf{q},\lambda} + \frac{1}{2} \right) \\ H_I &= \sum_{\mathbf{k},\mathbf{q},\lambda} g_{q,\lambda} c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger c_{\mathbf{k}\sigma} \left[a_{\mathbf{q},\lambda} + a_{-\mathbf{q},\lambda}^\dagger \right] \end{aligned} \quad (9.95)$$

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,

$$\epsilon(\mathbf{k}) = \epsilon_0(\mathbf{k}) + C_{\mu\nu} u_{\mu\nu}(\mathbf{x}) + \dots$$

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

$$\epsilon_F = \frac{1}{2m} \left(\frac{3\pi^2 N}{V} \right)^{\frac{2}{3}}. \quad (9.96)$$

When a portion of the lattice expands from $V \rightarrow V + dV$, 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

$$H_I = C \int d^3x \psi_{\sigma}^\dagger(\mathbf{x}) \psi_{\sigma}(\mathbf{x}) \vec{\nabla} \cdot \vec{\Phi} \quad C = -\frac{2}{3} \epsilon_F \quad (9.97)$$

The quantity C is often called the “deformation potential”. Now the displacement of the phonons was studied in Chapter 4. In a general model, it is given by

$$\Phi(\mathbf{x}) = -i \sum_{\mathbf{q},\lambda} \mathbf{e}_{\mathbf{q}}^\lambda \Delta x_{q,\lambda} \left[a_{\mathbf{q},\lambda} + a_{-\mathbf{q},\lambda}^\dagger \right] e^{i\mathbf{q}\cdot\mathbf{x}}$$

where we’ve introduced the shorthand

$$\Delta x_{q,\lambda} = \left(\frac{\hbar}{2MN_s\omega_{q,\lambda}} \right)^{\frac{1}{2}}$$

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 $\mathbf{e}_{\mathbf{q}}^\lambda$ is the polarization vector of the mode. For longitudinal phonons, for instance, $\mathbf{e}_{\mathbf{q}}^\lambda = \hat{q}$. The “ $-i$ ” in front 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 $(\mathbf{e}_{\mathbf{q}}^\lambda)^* = -(\mathbf{e}_{-\mathbf{q}}^\lambda)$) 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

$$\vec{\nabla} \cdot \Phi(\mathbf{x}) = \sum_{\mathbf{q},\lambda} \mathbf{q} \cdot \mathbf{e}_{\mathbf{q}}^\lambda \Delta x_{q,\lambda} \left[a_{\mathbf{q},\lambda} + a_{-\mathbf{q},\lambda}^\dagger \right] e^{i\mathbf{q}\cdot\mathbf{x}}$$

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

$$\begin{aligned} H_I &= C \int d^3x \psi_{\sigma}^\dagger(\mathbf{x}) \psi_{\sigma}(\mathbf{x}) \vec{\nabla} \cdot \vec{\Phi}(\mathbf{x}) \\ &= \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\lambda} c_{\mathbf{k}'\sigma}^\dagger c_{\mathbf{k}\sigma} \left[a_{\mathbf{q},\lambda} + a_{-\mathbf{q},\lambda}^\dagger \right] \frac{1}{V} \int d^3x e^{i(\mathbf{q}+\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} \times C \Delta x_{q,\lambda} (\mathbf{q} \cdot \mathbf{e}_{\mathbf{q}}^\lambda) \end{aligned}$$

$$= \sum_{\mathbf{q}, \lambda} g_{\mathbf{q}, \lambda} c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} [a_{\mathbf{q}, \lambda} + a^\dagger_{-\mathbf{q}, \lambda}] \quad (9.98)$$

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, $\sum_{\mathbf{q}} \equiv V \int_{\mathbf{q}} \rightarrow \int_{\mathbf{q}}$. 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 $N_s \rightarrow a^{-3}$ whenever we switch from discrete, to continuous integrals. With this understanding, we will use

$$g_{\mathbf{q}} = Cq \sqrt{\hbar a^3 / (2M\omega_{\mathbf{q}, \lambda})} \quad (9.99)$$

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,

$$\delta V(\mathbf{x}) = \sum_j \delta V_{\text{atomic}}(\mathbf{x} - \mathbf{R}_j^0 - \vec{\Phi}_j) = - \sum_j \vec{\Phi}_j \cdot \vec{\nabla} V_{\text{atomic}}(\mathbf{x} - \mathbf{R}_j^0)$$

we must replace interaction,

$$C \rightarrow V_{\text{atomic}}(\mathbf{q}) = \frac{1}{V_{\text{cell}}} \int d^3x V_{\text{atomic}}(\mathbf{x}) e^{-i\mathbf{q}\cdot\mathbf{x}}. \quad (9.100)$$

- 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

$$g_{\mathbf{k}'-\mathbf{k}, \lambda} \rightarrow g_{\mathbf{k}', \mathbf{k}, \lambda}.$$

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

$$D(\mathbf{q}, \tau - \tau') = -\langle T \phi_{\mathbf{q}}(\tau) \phi_{\mathbf{q}}(\tau') \rangle = T \sum_{i\nu_n} D(\mathbf{q}) e^{-i\nu_n(\tau - \tau')} \quad (9.101)$$

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where the propagator

$$D(q) = \frac{2\omega_{\mathbf{q}}}{(i\nu_n)^2 - (\omega_{\mathbf{q}})^2}$$

is denoted by the diagram

$$\begin{array}{c} \text{~~~~~} \\ (\mathbf{q}, i\nu_n) \end{array} = D(\mathbf{q}, i\nu_n) \quad (9.102)$$

The interaction vertex between electrons and phonon is denoted by the diagram

$$\begin{array}{c} \text{~~~~~} \\ \text{~~~~~} \\ \text{~~~~~} \end{array} \begin{array}{c} k+q \\ \mathbf{k} \\ q \end{array} = (i)^3 \times -g_{\mathbf{q}} = ig_{\mathbf{q}} \quad (9.103)$$

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

$$\begin{array}{c} \text{~~~~~} \\ \text{~~~~~} \end{array} \begin{array}{c} \text{~~~~~} \\ \text{~~~~~} \end{array} = (ig_{\mathbf{q}})^2 D(q) = -(g_{\mathbf{q}})^2 D(q) \quad (9.104)$$

so that the exchange of a boson induces an effective interaction

$$V_{\text{eff}}(\mathbf{q}, z) = g_{\mathbf{q}}^2 \frac{2\omega_{\mathbf{q}}}{(z)^2 - \omega_{\mathbf{q}}^2} \quad (9.105)$$

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

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