Physics 220- Fall 2017

Manybody Physics

Test-2
100 points, Time 90 mins
21 November, 2017

Solution.

1. Consider a free Fermi gas on N particles having spin half in 2-dimensions with area A, assuming free particle dispersion $\varepsilon_k = \hbar^2 k^2/(2m)$.

(a) Calculate the Fermi momentum and Fermi energy in terms of the particle density $n = N/A$. . . . [5]

We write the (aerial) density n as

$$n = \frac{2}{A}\sum_k \Theta(\varepsilon_F - \varepsilon_k) = \frac{2}{4\pi^2}\int dk_x\, dk_y \Theta(k_F^2 - k^2) = \frac{k_F^2}{2\pi},$$

where we used radial symmetry to write $dk_x\, dk_y = 2\pi\, kdk$.

(b) Assume now that the population in spins is disturbed so that $N_\uparrow = \frac{1+x}{2}N$ and correspondingly $N_\downarrow = \frac{1-x}{2}N$. Calculate the kinetic energy as a function of x. . . . [10]

We can solve this problem by using a simple idea, the density in the above problem (a) is the sum of the density of up and down spins, so that if the two had different values n_σ we would get

$$n_\sigma = \frac{k_{F\sigma}^2}{4\pi},$$

where $k_{F\sigma}$ is the Fermi momentum of spin σ electrons. As a test, notice that if we set equal densities for both and equal Fermi momenta, we are consistent with the result of (a). Now using $n_\sigma = n(1+\sigma x)/2$ (where $\sigma = \pm 1$)

$$k_{F\sigma} = \sqrt{2\pi n(1+\sigma x)}.$$

Now the total kinetic energy is given by

$$\begin{aligned} < T > &= \Sigma_{\sigma k}\, \varepsilon_k \Theta(k_{F\sigma} - k) = A\Sigma_\sigma \int k\frac{dk}{2\pi}\frac{\hbar^2 k^2}{2m}\Theta(k_{F\sigma} - k) \\ &= A\frac{\hbar^2}{2m}\Sigma_\sigma \frac{k_{F\sigma}^4}{8\pi} \\ &= N\varepsilon_F \frac{1+x^2}{2}. \end{aligned}$$

(c) In 2-dimensions consider the square lattice and sketch the Fermi surface for non interacting electrons in tight binding at half filling, with dispersion

$$\varepsilon_k = -2t(\cos(k_x) + \cos(k_y)),$$

and compare with the free electron Fermi surface $\varepsilon_k = \hbar^2 k^2/(2m)$ with the same number of particles. . . . [5]

We are trying to calculate μ using

$$\frac{n}{2} = \int_{-\pi}^{\pi} \frac{dk_x}{2\pi} \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} \Theta(\mu - \varepsilon_k), \tag{1}$$

with $n = 1$. We thus want the closed surface bounding half the area of the BZ defined as $-\pi \leq k_x, k_y \leq \pi$. The "baseball diamond" consisting of the interior region $\varepsilon_k \leq 0$ clearly has half the area. Hence this is the FS at half filling. *We have done this problem in detail in one of the HW's, and hence I am assuming familiarity with the FS. If you have not done the HW problem, this can be tedious in the exam.*

The free particle FS will be circular with the same area. Hence

$$\pi k_F^2 = \frac{1}{2} 4\pi^2. \tag{2}$$

2. Consider a cluster of 4 sites in the form of a square, with sites labeled by (1,2,3,4), and the pair creation operator

$$\eta^\dagger_{ab} = (c^\dagger_{a\uparrow} c^\dagger_{b\downarrow} - c^\dagger_{a\downarrow} c^\dagger_{b\uparrow}).$$

(a) Show (or argue) that $\eta^\dagger_{12}|0>$ gives a singlet pair at sites (a,b). . . . [10]

The wave function for this state will be

$$\phi_a(r_1)\phi_b(r_2)\left[\uparrow\downarrow - \downarrow\uparrow\right]$$

where ϕ_a, ϕ_b are the wave functions centered on sites a, b. This is clearly a singlet state.

(b) Calculate explicitly the non-zero elements of the state

$$|\Phi >= \frac{1}{2}(\eta^\dagger_{12} + \eta^\dagger_{23} + \eta^\dagger_{34} + \eta^\dagger_{41})^2 |0> .$$

. . . [10]

Here we need to recall from the class discussion that $\left(\eta^\dagger_{ab}\right)^2 = 0$, and hence we only need the cross terms which are 6 in number. The statement in red color is wrong since I am using the antisymmetrized η rather than the Dyson creation operator (one ote the two terms of $\eta^\dagger$. The true answer is $\left(\eta_{ab}^{\dagger}\right)^2 = 2n_{a\uparrow}n_{b\downarrow} + 2n_{a\downarrow}n_{b\uparrow}$, where $n_{a\sigma}$ is the number operator. Two terms vanish in the answer corresponding to two creators of same spin and site.

Remembering that $(A+B)^2 = A^2 + B^2 + \{A, B\}$ (think anticommutator), we get

$$\begin{aligned} 2|\Phi> &= \left[\{\eta_{12}^{\dagger}, \eta_{23}^{\dagger}\} + \{\eta_{23}^{\dagger}, \eta_{34}^{\dagger}\} + \{\eta_{34}^{\dagger}, \eta_{41}^{\dagger}\} + \{\eta_{41}^{\dagger}, \eta_{12}^{\dagger}\}\right] \\ &\left[+(\eta_{12}^{\dagger})^2 + (\eta_{23}^{\dagger})^2 + (\eta_{34}^{\dagger})^2 + (\eta_{41}^{\dagger})^2 + 2\eta_{12}^{\dagger}\eta_{34}^{\dagger} + 2\eta_{23}^{\dagger}\eta_{41}^{\dagger}\right] |0> . \end{aligned}$$

The last two terms have no common sites in the product and hence there is no need to antisymmetrize.

(c) Consider the operator

$$P(g) = e^{-g\sum_{i=1}^{4} n_{i\uparrow}n_{i\downarrow}}.$$

Show that this leaves singly occupied states untouched and suppresses double occupancy by a certain g dependent factor. . . . [10]

This is the famous Gutzwiller operator, which has been of fundamental importance. We know that $n_{i\uparrow}n_{i\downarrow}$ is one of the operators that is invariant under squaring, or in fact taking any non-zero power. Hence we can immediately write

$$P(g) = \prod_{i=1}^{4}\left(1 + (e^{-g} - 1)n_{i\uparrow}n_{i\downarrow}\right) .$$

Clearly this operator seeks out and suppresses doubly occupied sites by a factor e^{-g} which is small if $g \gg 0$.

(d) Calculate

$$|\Psi >= \lim_{g\to\infty} P(g)|\Phi >,$$

where $|\Phi>$ was defined in (b) above. . . . [10]

This is easy since only the last two terms have non-overlapping terms. Hence

$$|\Psi >= \left[\eta_{12}^{\dagger}\eta_{34}^{\dagger} + \eta_{23}^{\dagger}\eta_{41}^{\dagger}\right] |0> . \quad (3)$$

This also happens to be a well known wave function, the exact ground state for the Heisenberg antiferromagnet on the 4 site cluster. P W Anderson was inspired by this wave function and generalized it to the so-called resonating valence bond state.

$$|RVB >= \lim_{g\to\infty} P(g)|\Phi_0 > \quad (4)$$

where $|\Phi_0>$ is the free Fermi ground state (band state).

3. Consider the Hubbard model in the very simple atomic limit where the kinetic energy vanishes. Thus we can ignore the site indices and consider a single site where the H is given as

$$H = -\mu \sum_{\sigma} n_{\sigma} + U n_{\uparrow} n_{\downarrow}.$$

(a) Calculate the partition function Z exactly. ...[10]

This is quite simple.

$$Z = 1 + 2e^{\beta\mu} + e^{2\beta\mu} e^{-\beta U}.$$

The factor of 2 in the second term comes from the two spin directions.

(b) In this case calculate the two time independent correlation functions

$$k_1 =< c_{\uparrow} c_{\uparrow}^{\dagger} >, \quad k_2 =< c_{\uparrow}^{\dagger} c_{\uparrow} >$$

in terms of μ, U and T. ...[15]

Let us calculate k_2 and find $k_1 = 1 - k_2$ (using the ACR).

$$k_2 = \frac{1}{Z}(e^{\beta\mu} + e^{\beta\mu} e^{-\beta U}),$$

where the first term comes from single occupancy of the up spin and the second one from double occupancy. Hence

$$k_1 = \frac{1}{Z}(1 + e^{\beta\mu}).$$

The interpretation of the answer is fun, the first term (1) comes from vacuum where we can add the up electron, and the second from occupied down spin state where we can add the up spin using the creation operator.

(c) Calculate the average double occupancy

$$d =< c_{\uparrow}^{\dagger} c_{\uparrow} c_{\downarrow}^{\dagger} c_{\downarrow} >$$

in terms of μ, U and T. Show that $d \to 0$ as $U \to +\infty$. ...[15]

This is as simple as (b).

$$d = \frac{1}{Z}(e^{2\beta\mu} e^{-\beta U})$$

Only the doubly occupied term contributes to d.