Concepts of condensed matter physics - Exercise #3

Spring 2020

Due date: 29/06/2020

1. **Path integral formulation for free particles**

Consider a gas of free particles with energies ε_a (where the index a labels the single-particle eigenvalues) and chemical potential μ. In this question you will use the path integral formalism to find thermodynamic properties of this system. Notice that while the path integration in this case is much more complicated compared to the alternatives, the techniques you will use here are important in more interesting scenarios. (Consult "Condensed matter field theory" by A. Altland and B. Simons chapter 4).

a. Write the general form of the total particle number, the total energy, and the free energy characterizing this system in terms of the Fermi (or Bose-Einstein) distribution (without using the path integral formalism).

b. Write the partition function as a path integral and perform the functional integration. Use this to write the free energy, the particle number, and the energy of the system. For now you can write these as sums over a and the Matsubara frequencies.

c. To find the particle number and energy from the above sums, write them in the form $\sum_n h(\omega_n)$. Notice that the sum is of the form $\sum_n \frac{C}{i\omega_n - \varepsilon}$, which actually doesn't converge. To take care of that, write it in the form $\sum_n \frac{C}{i\omega_n e^{-i\omega_n\delta} - \varepsilon}$, where δ is a positive infinitesimal (can you think of its physical origin?). Show that you can write the sum as a contour integral $\frac{\zeta}{2\pi i}\oint g(z)h(-iz)dz$, with $g(z) = \frac{\beta}{e^{\beta z} - \zeta}$ and the contour shown in Fig. (a), where the crosses represent the poles of the function g. Show that one can deform this contour to that shown in Fig. (b), where the crosses which are not on the imaginary line represent the poles of the function $h(-iz)$. Use this to calculate the total number of particles and the energy of the system.

d. To find the free energy, write it again in the form $\sum_n h(\omega_n)$ and use the same trick to transform it to a contour integral. Note that now the function $h(-iz)$ has a branch cut, so special care must be taken in deforming the contour. Also, ignore the infinite constant contribution coming from the contour at infinity (does it affect any physical observable?).

(a)   (b)
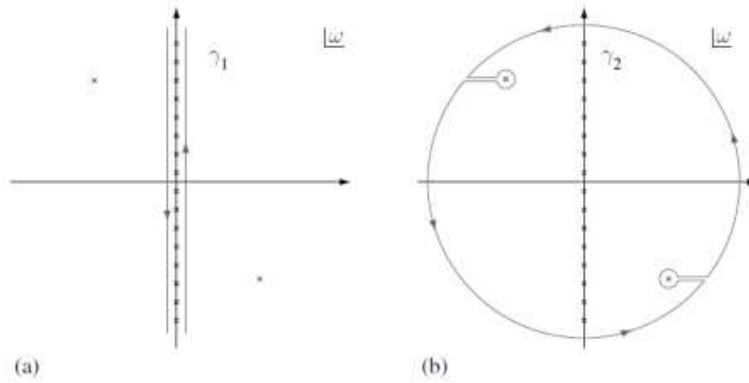
2. Itinerant ferromagnetism in weakly interacting Fermi fluids (The Stoner instability)

Consider the following Hamiltonian of interacting Fermions

$$\hat{H} = \int d^3x \left[\sum_{s=\uparrow\downarrow} c_s^+(x) \left(-\frac{\nabla^2}{2m} - \mu \right) c_s(x) + g\, c_\uparrow^+(x)c_\downarrow^+(x)c_\downarrow(x)c_\uparrow(x) \right]$$

Here $c_s(x)$ annihilates a fermion with spin $s = \uparrow, \downarrow$ at point x, μ is the chemical potential and g is the strength of contact (delta function) interaction between the two different spin state densities. In this exercise you will examine three independent approaches to performing mean field theories.

a. Write the interactions as $\frac{g}{4}(n^2 - 4s^2)$, where $n = n_\uparrow + n_\downarrow$ and $s = \frac{1}{2}(n_\uparrow - n_\downarrow)$. Perform the Hubbard-Stratonovich (HS) transformation and introduce two auxiliary fields ρ, m. Doing this, you will obtain a theory of non-interacting Fermions coupled to Bosonic magnetization and density fields.

b. Find the saddle point of the action at zero temperature by equating the functional derivative of the action S with respect to the auxiliary fields to zero. Obtain an integral equation to determine the average values of the auxiliary fields by assuming that they are fixed in space and time and by taking the expectation value over the Fermionic fields.

c. Solve the equation obtained in b. by linearizing it with respect to m. What is the critical value $g = g_c$ above which the magnetization develops a finite expectation value? Express your result in terms of an effective chemical potential (given that the number of particles is fixed n_0). What is the critical exponent β defined by the singularity of the average magnetization near the transition $|\langle m \rangle| \sim |g - g_c|^\beta$?

d. To gain more intuition we will now obtain the same result using mean-field. Starting from the Hamiltonian above, substitute the electrons spin and density with a mean-field $s \equiv M + \delta s, n = n_0 + \delta n$ where M and n_0 are the mean-field values. Neglect terms of order $O(\delta s^2), O(\delta n^2)$, and obtain a quadratic Hamiltonian. In a self-consistent manner compute the expectation values of s, n using this quadratic Hamiltonian and obtain the same integral equation as in section c.

e. Finally, we would like to obtain this result in yet another way: the variational approach. Compute the expectation value of the full interacting Hamiltonian (above) using the ground state of the mean-field Hamiltonian from section d. Minimize this expectation value with respect to the variational parameters M, n_0 and obtain the same equation again.

f. Bonus: In the previous sections we performed the mean field approximation in the exchange and direct channels, taking a specific combination of the two channels and neglecting the Cooper channel. Alternatively, we can also have different combinations of the direct and exchange channels, or assume the term $c_\uparrow^+(x)c_\downarrow^+(x)$ (Cooper channel) is weakly fluctuating. These possibilities were not accounted for in the analysis above. How would you generalize the mean field treatment of previous sections such that all the channels are taken into account?

3. Debye-Waller factor of low dimensional crystals and the Mermin-Wagner theorem

(Consult the L and N appendices of "Solid State Physics" By Neil Ashcroft and David Mermin). In this question we will show that in low dimensional systems the fluctuations associated with the Goldstone modes of a crystal (a.k.a. phonons) diverge and destroy the long range order even if they are small on the microscopic scale. To see that, we will perform a full quantum mechanical treatment of the problem. Like we did in class, we will first assume that the fluctuations are small. This will allow us to derive an effective theory. Using this theory we will find that in low dimensions the fluctuations can actually be very large when we look at large distances, in conflict with the original assumption.

To be specific, we consider the Hamiltonian of ions in a cubic crystal phase of general dimension d

$$H = \sum_{j=1}^{N} \frac{P_j^2}{2M} + \sum_{\langle ij \rangle} V(r_i - r_j)$$

The $\langle ij \rangle$ brackets denote summation over nearest neighbors.

Let us denote the classical ground state positions of the ions by $\{R_j\}_{j=1}^{N}$. We can expand the potential $V(r)$ up to quadratic order in deviations around the ions' classical ground state positions, i.e. we take $r_j = R_j + u_j$ where $\langle |u_j| \rangle \ll a$, and a is the inter-ion distance. A typical low-energy Hamiltonian then assumes the form

$$H = \sum_i \frac{P_i^2}{2M} + \sum_{\langle ij \rangle} \frac{K}{2}(\boldsymbol{u}_i - \boldsymbol{u}_j)^2,$$

which is nothing but an array of coupled harmonic oscillators.

a. Diagonalize the Hamiltonian using the ladder operators in quasi-momentum space, a_k, such that it takes the simple form $H = \sum_k \omega_k \left(a_k^+ a_k + \frac{1}{2}\right)$. Plot the Goldstone mode dispersion within the first Brillouin zone.

   Comment: To understand if the system maintains long-range order (LRO) we consider the density-density correlation function, given by

   $$C(\boldsymbol{r}, \boldsymbol{r}'; t, t') \equiv \langle \rho(\boldsymbol{r}, t) \rho(\boldsymbol{r}', t') \rangle$$

   where $\langle O \rangle = \frac{Tr[e^{-\beta H}O]}{Tr e^{-\beta H}}$ denotes quantum averaging in a thermal ensemble, such that $\langle a_k^+ a_k \rangle = \frac{1}{e^{\beta \omega_k} - 1}$. Here the density operator is defined as follows

   $$\rho(\boldsymbol{r}, t) \equiv \sum_{j=1}^N \delta\left(\boldsymbol{r} - \boldsymbol{r}_j(t)\right)$$

   If LRO exists throughout the system we expect that in the limit $|\boldsymbol{r} - \boldsymbol{r}'| \to \infty$ the function $C(\boldsymbol{r}, \boldsymbol{r}'; 0,0)$ will have a finite amplitude modulation at the crystal periodicity. The physics behind this notion is rigidity, namely, if we perturb an ion at $\boldsymbol{r}$ then the ion at $\boldsymbol{r}'$ will move in correlation with its motion (even if $|\boldsymbol{r} - \boldsymbol{r}'| \to \infty$).

b. Use the space and time translational invariance of the correlation function (i.e. $C(\boldsymbol{r}, \boldsymbol{r}'; t, t') = C(\boldsymbol{r} - \boldsymbol{r}'; t - t')$)) to show that it's Fourier transform is given by

   $$C(\boldsymbol{q}, \boldsymbol{k}; \omega, \omega') = V \delta_{\boldsymbol{k}, \boldsymbol{q}} (2\pi) \delta(\omega + \omega') S(\boldsymbol{q}, \omega),$$

   where the Fourier transform is defined as

   $$C(\boldsymbol{q}, \boldsymbol{k}; \omega, \omega') = \int d^d r \, d^d r' \, dt \, dt' \, C(\boldsymbol{r}, \boldsymbol{r}'; t, t') e^{i(\boldsymbol{q} \cdot \boldsymbol{r} + \boldsymbol{k} \cdot \boldsymbol{r}' + \omega t + \omega' t')}$$

   and

   $$S(\boldsymbol{q}, \omega) = \frac{1}{V} \sum_{jj'} \int dt \, e^{-i\omega t} \langle e^{-i\boldsymbol{q} \cdot \boldsymbol{r}_j(t)} e^{i\boldsymbol{q} \cdot \boldsymbol{r}_{j'}(0)} \rangle$$

   Note that this function is known as the *dynamic structure factor*. Do not forget that we are working in a finite size system where $V = Na^d$.

c. Use the identity $\langle e^{A+B} \rangle = e^{1/2\langle (A+B)^2 \rangle}$ to show that you can write the dynamic structure factor $S(q, \omega)$ in the form

$$S(q, \omega) = \frac{e^{-2W}}{a^d} \sum_{j=1}^{N} e^{iq \cdot R_j} \int dt e^{-i\omega t} e^{\langle (q \cdot u_0)(q \cdot u_j(t)) \rangle}$$

where $W \equiv \frac{1}{2}\langle (q \cdot u_0)^2 \rangle$ is known as the *Debye-Waller* factor.

d. Compute the Debye-Waller factor for a general dimension d. For simplicity assume that the phonons have a linear dispersion, which is cutoff by the Debye frequency ω_D set by the width of the dispersion band.

   Comment: To obtain the long range modulations we take the term in the exponent to be unity such that the sum over j can be performed (the idea is that delta functions in q-space translate to pure long-range modulations in real space). In such a case one would obtain

$$S(q, \omega) \propto e^{-2W} \sum_{G} \delta_{qG}$$

   where G are the reciprocal lattice vectors. This result implies that for very low frequencies the delta functions are weighted by Ne^{-2W}.

e. Show that in one dimension W diverges for all temperatures. Is zero temperature different?
f. Show that in two-dimensions W diverges at finite temperatures.
g. Show the similarity between the one-dimensional case at zero temperature and the two-dimensional case at finite temperatures. Can you explain this in terms of path integrals?