Concepts of condensed matter physics - Exercise #1

Spring 2016

Due date: 12/04/2016

1. Path integral formulation for free particles

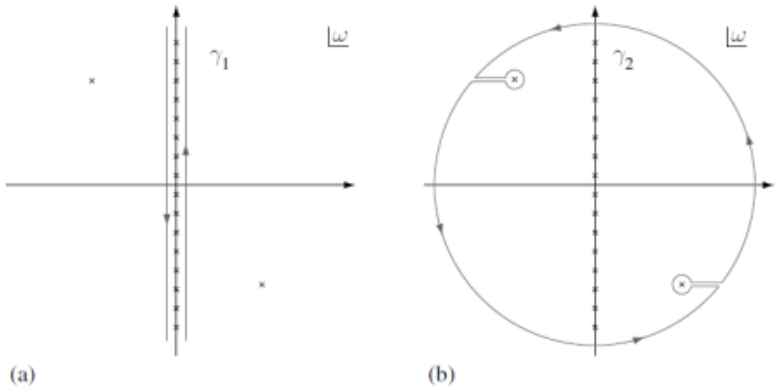
Consider a gas of free particles with energies ε_a (where the index a labels the single-particle eigenvalues) and chemical potential μ. In this question you will use the path integral formalism to find thermodynamic properties of this system. Note that while the path integration in this case is much 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 $\sum_n h(\omega_n)$. Note 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. <u>Itinerant ferromagnetism in weakly interacting Fermi fluids</u> (The Stoner instability)

Consider the following Hamiltonian of interacting Fermions

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

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? 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. <u>Bonus</u>: 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. **Spin-wave dispersion** (Consult "Interacting Electrons and Quantum Magnetism" by A. Auerbach pages 123 - 126)**.** In this question you are asked to derive the spin-wave dispersion of the two-dimensional Heisenberg model on a square lattice with antiferromagnetic coupling (i.e. $J > 0$). The Hamiltonian of such a model is given by

$$H = J \sum_{\langle ij \rangle} \left[S_i^z S_j^z + \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)\right]$$

where $S^+ = (S^x + S^y)/2$ and $S^- = (S^+)^+$ are the spin raising and lowering operators and $S^{x,y,z}$ are the spin-half operators which are arranged on a square lattice. The $\langle ij \rangle$ brackets denote summation over nearest neighbors.

a. Separate the lattice into two sub-lattices, A and B, such that all the neighbors of an A site are B's and vice versa. Now take $\langle S_j^z \rangle = \eta(j)$ where $\eta(j) = 1$ if $j \in A$ and $\eta(j) = -1$ if $j \in B$. What is the ground state-energy given by this solution?

b. Show that the mean-field solution you have obtained is not an eigen-state of the Hamiltonian, and thus is not the true ground state.

c. Now let us refine the solution by accounting for quantum fluctuations. First apply a rotation of π about the x axis to all spins on sub-lattice B $\boldsymbol{S}_j \rightarrow \tilde{\boldsymbol{S}}_j$ (the idea is that we expand the Hamiltonian around the mean-field solution, where we have assumed that the spins are aligned along the z direction and anti-parallel to all their nearest neighbors). Now let us assume that all spins are fluctuating weakly around $\langle \tilde{S}_i^z \rangle \approx \frac{1}{2}$, such that we may introduce the Holstein-Primakoff bosons

$$S^z = \frac{1}{2} - n_b$$
$$S^+ = \sqrt{1 - n_b}\, b$$
$$S^- = b^+ \sqrt{1 - n_b}$$

where $n_b = b^+ b$. Apply this transformation

d. Diagonalize the Bosonic theory using a Bogoliubov transformation. Plot the spin-wave dispersion schematically. (note that in the limit of weak fluctuations $\langle n_b \rangle \ll 1$).

e. In class you have derived the spin-dispersion of the ferromagnetic model (i.e. $j < 0$). Discuss the difference in the long wave-length dependence?