Concepts of condensed matter physics - Exercise #2

Spring 2021

Due date: 09/06/2021

1. t/U expansion of the Hubbard Hamiltonian

In class we have derived the low energy effective Hamiltonian of the Hubbard model in the limit $U \gg t$ at half filling using degenerate perturbation theory. To order $\frac{t}{U^2}$ we found the Heisenberg model with $J = \frac{4t^2}{U}$. In this question you will take a different route to expand the Hubbard Hamiltonian in orders of $\frac{t}{U}$ and recover the Heisenberg model once again to the appropriate order at half filling. For simplicity we will use a single index i to label the sites of a d dimensional lattice by some unspecified order. The Hubbard Hamiltonian is:

$$H = T + V = -t \sum_{i,j,s} N_{ij} c_{i,s}^{\dagger} c_{j,s} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

where $N_{ij} = 1$ if i and j are nearest neighbors and zero otherwise.

a. Write the kinetic part, $T = -t \sum_{i,j,s} N_{ij} c_{i,s}^{\dagger} c_{j,s}$, as a sum over three parts: T_{-1} which decreases the number of double occupied sites by 1, T_0 which keeps the number of doubly occupied sites unchanged, and T_1 which increases the number of doubly occupied sites by 1. Give explicit expressions for the various T_m in terms of the creation and annihilation operators $c^{\dagger}$ and c, the electron number operator n and the hole number operator $h = 1 - n$. ***Hint:*** multiply T by $\left(n_{i,\bar{s}} + h_{i,\bar{s}}\right) = 1$ from the left and by $\left(n_{j,\bar{s}} + h_{j,\bar{s}}\right) = 1$ from the right.

b. Calculate the commutator of the interaction V with the various kinetic terms T_m. What is the meaning of the result you find?

c. We wish to find a unitary operator S with which to transform the Hamiltonian such that it does not connect states with different numbers of doubly occupied sites. Expand the transformed Hamiltonian $H' = e^{iS} H e^{-iS}$ in a series of commutators (the Schrieffer-Wolff transformation) and show that choosing $iS = \frac{1}{U}(T_1 - T_{-1}) + O\left(\frac{t^3}{U^2}\right)$ eliminates T_1 and T_{-1} from the Hamiltonian. What is the resulting H' to this order? Write it both in terms of V and the various T_m and in terms of the creation and annihilation operators $c^{\dagger}$ and c, the electron number operator n and the hole number operator h.

d. Now we will specialize to the subspace of states at half filling with no doubly occupied states, i.e., the low energy subspace in the large U limit. Denoting this subspace be L what are $T_0|\psi\rangle_L$, $T_{-1}|\psi\rangle_L$ and $V|\psi\rangle_L$? In light of these results, rewrite the simplified H' when acting on this subspace.

e. Analyze the form of H' you obtained and rewrite it in terms of the spin operators: $S^z = \frac{1}{2}[|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|]$, $S^+ = |\uparrow\rangle\langle\downarrow|$, and $S^+ = |\downarrow\rangle\langle\uparrow|$, as we did in the tutorial.

It is possible, albeit complicated, to keep constructing iS to higher orders in order to keep eliminating T_1 and T_{-1} to higher orders in H'. At half filling the resulting H' acting on the low energy subspace L will result in a spin model to any order in $\frac{t}{U}$, but the higher order terms in H' will involve more and more spins. Therefore, it is wise to start with the Heisenberg model and analyze various symmetry allowed spin terms on top of it instead.

2. Path integral formulation for free particles

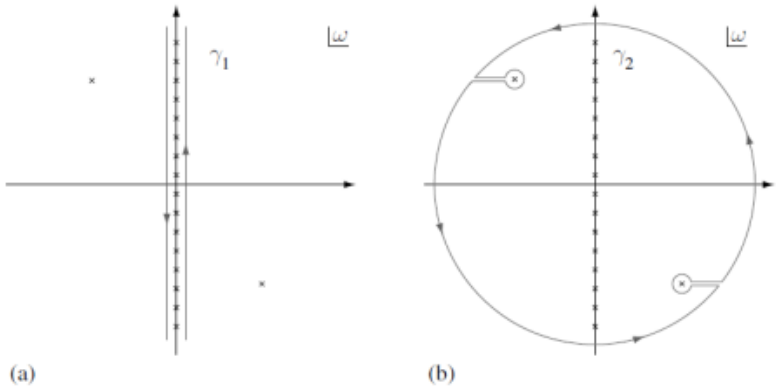
Consider a gas of free particles with energies ε_a (where the index a labels the single-particle eigenvalues) and chemical potential μ. In this question you will use the path integral formalism to find thermodynamic properties of this system. Note that while the path integration in this case is much 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?).



3. <u>Itinerant ferromagnetism in weakly interacting Fermi fluids</u> (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?