Concepts in Condensed Matter Physics: Exercise 1

Due date: 17/05/22

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 $\frac{t^2}{U}$ 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:

$$H = T + V = -t \sum_{i,j,\sigma} N_{i,j} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \ , \tag{1}$$

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

1. Write the kinetic part, $T = -t \sum_{i,j,\sigma} N_{i,j} c^\dagger_{i,\sigma} c_{j,\sigma}$, 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 $(n_{i,\bar{\sigma}} + h_{i,\bar{\sigma}}) = 1$ on the left and by $(n_{j,\bar{\sigma}} + h_{j,\bar{\sigma}}) = 1$ on the right.

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

3. 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 $iS = \frac{1}{U}(T_1 - T_{-1}) + O\left(t^3/U^2\right)$ eliminates T_1 and T_{-1} from $H = V + T_0 + T_1 + T_{-1]}$. What is the resulting H' to this order, $O(t^3/U^2)$? 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 $h = 1 - n$.

4. 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.

5. Analyze the form of H' you obtained and rewrite it in terms of the spin operators: $S^z = \left[\frac{1}{2} |\uparrow\rangle \langle\uparrow| - |\downarrow\rangle \langle\downarrow|\right]$, $S^+ = |\uparrow\rangle \langle\downarrow|$ and $S^- = (S^+)^\dagger$, 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 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

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

The $\langle i, j \rangle$ brackets denote summation over nearest neighbors.

1. 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 $\langle S_j^z \rangle = \eta(j)$, with $\eta(j) = 1$ if $j \in A$ and $\eta(j) = -1$ if $j \in B$. What is the energy of this configuration?

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

3. 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, $\vec{S}_j \to \tilde{\vec{S}}_j$ (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 $\left\langle \tilde{S}_i^z \right\rangle \approx \frac{1}{2}$, such that we may introduce the Holstein-Primakoff bosons

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

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

$$S^- = b^\dagger \sqrt{1 - n_b},$$

where $n_b = b^\dagger b$. Apply this transformation to the Hamiltonian.

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

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