PHYSICS 320: Problem Set No. 4
Due: Fri. Oct. 29 2010

1. For the Hubbard model

$$H = \sum_{i\neq j,\sigma} -t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.} + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

show that the operators for total number of up spin electrons $M_\uparrow$ and downspin electrons $M_\downarrow$ commute with the Hamiltonian and hence so does the operator for total number of electrons M. The energy eigenvalues $\{E(m_\uparrow, m_\downarrow)\}$, can be labelled by $m_\sigma = M_\sigma/N$, where N is the number of lattice sites.

   (a) Now, assume that the lattice is bipartite and the hopping $t_{ij} = t$ for nearest neighbours and zero otherwise. Show that

   $$\{E(1-m_\uparrow, 1-m_\downarrow)\} = \{E(m_\uparrow, m_\downarrow)\}$$

   up to an additive constant. What is this constant? (*Hint: Make a suitable transformation of the electron creation and annihilation operators* $c^\dagger_{i\sigma}$ *and* $c_{i\sigma}$ *which maps the Hamiltonian back onto itself up to an additive constant but with densities* $1-m_\uparrow$ *and* $1-m_\downarrow$ *instead of* $m_\uparrow$ *and* $m_\downarrow$*.*)

   (b) Now consider two ways of modifying the Hamltonian of part (a): 1) By adding a term $-t' \sum_{\langle il\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma}$+h.c. and 2) by adding a term V$\sum_{\langle il\rangle} n_i n_l$, where $n_i = \sum_\sigma n_{i\sigma}$. In both cases $\langle il\rangle$ denote next nearest neighbours. In which of these cases is

   $$\{E(1-m_\uparrow, 1-m_\downarrow)\} = \{E(m_\uparrow, m_\downarrow)\}$$

   up to an additive constant?

2. A two-site Hubbard model has the Hamiltonian

$$H = -t \sum_\sigma c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma} + U\left[n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow}\right].$$

If there are two electrons and $|t|/U \ll 1$, show that second order perturbation theory generates a Hamiltonian of the form $H = J\mathbf{S}_1 \cdot \mathbf{S}_2$ between the spins of the electrons on the two sites. What is the value of J and its sign?

The above simple two site problem demonstrates how one obtains a spin 1/2 Heisenberg model from a half-filled Hubbard model in the limit of small $|t|/U$ using perturbation theory. Let us now consider a spin 1/2 Heisenberg model

$$H_H = J \sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j,$$

on a $2N \times 2N$ square lattice with periodic boundary conditions. Here $\langle ij\rangle$ are nearest neighbours. Assume J can have either sign.

   (a) Show that the ferromagnetic state with all spins pointing in the same direction is an eigenstate of H_H. In particular show that when $J < 0$, this state is the ground state.

   (b) Now, show that the Neel state is not an eignestate of H_H.

Despite the fact the Neel state is not an eigenstate of H_H for any finite N, it can be shown (rather non-trivially) that it is indeed the ground state as $N \to \infty$ for $J > 0$.

3. As was shown in class a consideration on ferromagnetism in the Hubbard model within Hartree-Fock theory yields the following energy for the ground state.

$$E(m) = \sum_{\mathbf{k}} \left[(\epsilon_{\mathbf{k}} - e_{\mathbf{k}} U m)\, n^+_k + (\epsilon_{\mathbf{k}} + e_{\mathbf{k}} U m)\, n^-_k\right] + UNm^2,$$

where $\epsilon_{\mathbf{k}}$ is the band dispersion, m, the ferromagnetic order parameter ($|m| < 1$), $n^\pm_k$ the occupancies of states in the two magnetic subbands and $e_{\mathbf{k}} = \pm 1$. Further

$$m = \frac{1}{2N} \sum_{\mathbf{k}} e_{\mathbf{k}} \left(n^+_{\mathbf{k}} - n^-_{\mathbf{k}}\right).$$

(a) Assume the band dispersion is free electron like $\epsilon_{\mathbf{k}} = \hbar^2|\mathbf{k}|^2/2m$ and that $\mathbf{k}$ takes on continuous values from $+\infty$ to $-\infty$. Show that at $T = 0$ for certain values of the density of electrons n, the paramagnetic state has the lowest energy while for others a ferromagnetic state with $m \neq 0$ has the lowest energy. Show that the transition from paramagnet to ferromagnet as a function of n is continuous. At what value of n does it occur?

(b) Is the ferromagnetic state the ground state for high or low densities? Is this similar or different compared to the case of the jellium model you encountered in problem # 4 of problem set #2? Why?

4. Now, consider the case of spin density wave (SDW) order in the Hubbard model in Hartree-Fock theory. The energy of the ground state as a function of the SDW order parameter $m_{\mathbf{q}}$ is

$$E(m_{\mathbf{q}}) = \sum_{\mathbf{k}} \left[E^+_{\mathbf{k}} n^+_k + E^-_{\mathbf{k}} n^-_k \right] + UNm^2_{\mathbf{q}},$$

where

$$E^{\pm}_{\mathbf{k}} = \frac{\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k+q}}}{2} \pm e_{\mathbf{k}} \sqrt{\left(\frac{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+q}}}{2}\right)^2 + U^2 m^2_{\mathbf{q}}}.$$

Here $\epsilon_{\mathbf{k}}$ is the band dispersion and $e_{\mathbf{k}} = \pm 1$. Determine the condition for a continuous transition to take place from a paramagnetic ($m_{\mathbf{q}} = 0$) state to a SDW state. Do this by expanding the energy to second order in the order parameter and determining when the relevant coefficient changes sign.

5. Consider the Hubbard model

$$H = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

without the hopping term and $U > 0$.

(a) At $T = 0$, the chemical potential is the energy required to add a particle to the system, i.e. $\mu = E(N + 1) - E(N)$, where $E(N)$ is the energy of the system with N particles. Calculate the chemical potential as a function of the filling n.

(b) Now consider $T \neq 0$. Once again calculate μ as a function of n. It will help to use the partition function in the grand canonical ensemble. Show that you obtain the same value of μ as part (a) in the limit $T \to 0$.