Problem set 3

1. **Magnetic ordering in metals: paramagnetic vs. ferromagnetic ground states**: Consider the interacting electron Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{1}{2V} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\mathbf{q}} \sum_{\sigma,\sigma'} v(\mathbf{q}) \mathbf{c}^{\dagger}_{\mathbf{k}-\mathbf{q},\sigma} \mathbf{c}^{\dagger}_{\mathbf{k}'+\mathbf{q},\sigma'} \mathbf{c}_{\mathbf{k}',\sigma'} \mathbf{c}_{\mathbf{k},\sigma}$$

with the term $\mathbf{q} = \mathbf{0}$ included. Here, $V = L^d$ is the total volume of the system (in d dimensions), and the total number of electrons is N.

Consider the following types of possible states:

(i) a ferromagnetic state with all spins up,

$$|FM\rangle = \prod_{|\mathbf{k}|<\mathbf{k_F}} c^{\dagger}_{\mathbf{k},\uparrow} |0\rangle$$

(ii) a paramagnetic state with half of the spins up and half of the spins down:

$$|PM\rangle = \prod_{|\mathbf{k}|<\mathbf{k_F},\sigma} c^{\dagger}_{\mathbf{k},\sigma} |0\rangle$$

Find the total energy of the system $\langle \mathcal{H} \rangle$ for both types of states. Considering a short-range repulsive potential $v(\mathbf{r}) = \mathbf{G}\delta(\mathbf{r})$ with Fourier transform $v(\mathbf{q}) = \mathbf{G}$, find the critical density n_c at which a transition from a ferromagnetic to a paramagnetic state will occur for $d = 1$.

If you want to (not marked), repeat the calculations in $d = 3$, for $v(q) = 4\pi/q^2$, with the $q = 0$ term now excluded from the Hamiltonian. Which state is favored at low concentrations in this case, and why?

2. **Equivalence between the Hubbard model at half-filling, and an antiferromagnetic Heisenberg Hamiltonian**: Consider the Hubbard Hamiltonian $\mathcal{H} = \mathcal{H}_0 + V$, where

$$\mathcal{H}_0 = \sum_{\substack{i \neq j \\ \sigma}} t_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} \qquad \text{and} \qquad V = U \sum_i a^{\dagger}_{i\uparrow} a_{i\uparrow} a^{\dagger}_{i\downarrow} a_{i\downarrow}$$

Here, $t_{ij} = t^*_{ji}$ is the hopping amplitude from site i to site j and U is the on-site Coulomb repulsion energy. We assume that the sites form a lattice with a total of N sites, and that the total number of electrons is also N (half-filling).

Consider the perturbation treatment in the limit $U >> |t_{ij}|$. In this case, we have a 2^N manifold of degenerate eigenstates of V, with total energy $E_0 = 0$, of the general form

$$|\sigma_1, \sigma_2, ..., \sigma_N\rangle = a^{\dagger}_{1,\sigma_1} a^{\dagger}_{2,\sigma_2} ... a^{\dagger}_{N,\sigma_N} |0\rangle \qquad (1)$$

Any other states with N electrons will have at least one site containing two electrons and one site without any electrons, so their energies are U or higher, and we neglect them. The perturbation from $\mathcal{H}_0$ now lifts the degeneracy between these 2^N states with one-electron per site. Second order Rayleigh-Schrodinger perturbation theory leads to the energy shift

$$E^{(2)} = \sum_{\alpha} \frac{\langle \chi_0 | \mathcal{H}_0 | \chi_\alpha \rangle \langle \chi_\alpha | \mathcal{H}_0 | \chi_0 \rangle}{E_0 - E_\alpha}$$

Here, $|\chi_0\rangle$ is any ket vector chosen from the unperturbed basis (1), and $|\chi_\alpha\rangle$ is a state which has one site containing both an up and down spin, one site with no electrons, and all other sites singly occupied. Clearly, $E_\alpha = \langle\chi_\alpha|V|\chi_\alpha\rangle = U$ for any $|\chi_\alpha\rangle$.

This means that the energy shift $E^{(2)}$ of any singly-occupied state $|\chi_0\rangle$ is the same as that obtained from an effective Hamiltonian $\mathcal{H}_{eff} = -\mathcal{H}_0^2/U$.

Prove that the action of $\mathcal{H}_{eff}$ on the subspace generated by the singly-occupied vectors of type (1) is identical to the Heisenberg Hamiltonian

$$\mathcal{H}_{Heisenberg} = \sum_{i\neq j} J_{ij}\left(\vec{s}_i\cdot\vec{s}_j - \frac{1}{4}\right)$$

where $\vec{s}_i = \frac{1}{2}\sum_{\alpha,\beta} a^\dagger_{i\alpha}\vec{\sigma}_{\alpha\beta}a_{i\beta}$ is the spin operator for site i, with $\vec{\sigma}$ being the Pauli matrices. What is the value of J_{ij} for this equivalence to hold?

3. **Mean-field solution for half-filled, 1D Hubbard model**: Consider the 1D Hubbard Hamiltonian

$$\mathcal{H} = -t\sum_{i,\sigma}\left(c^\dagger_{i,\sigma}c_{i+1,\sigma} + h.c.\right) + U\sum_i c^\dagger_{i,\uparrow}c_{i\uparrow}c^\dagger_{i,\downarrow}c_{i\downarrow}$$

where $i = 1, 2, ..., N$ indexes the sites of the 1D chain (we assume periodic boundary conditions). We want to find a self-consistent Hartree-Fock solution for the half-filled chain, for which the number of electrons equals the number of sites, N. We assume N to be an even number.

Using any method you like, find the Hartree-Fock component of the Hamiltonian,

$$\mathcal{H} = \sum_n E_n a^\dagger_n a_n + ...$$

where

$$a_n = \sum_{i,\sigma}\phi^*_n(i\sigma)c_{i\sigma}; \qquad a^\dagger_n = \sum_{i,\sigma}\phi_n(i\sigma)c^\dagger_{i\sigma}$$

etc. You should find that in terms of the spinors

$$\phi_n(i) = \begin{pmatrix}\phi_n(i,\uparrow)\\ \phi_n(i,\downarrow)\end{pmatrix}$$

the self-consistent equations can be written as:

$$E_n\phi_n(i) = -t\left[\phi_n(i+1) + \phi_n(i-1)\right] + U\left[\frac{Q(i)}{2} - \vec{\sigma}\cdot\vec{S}(i)\right]\phi_n(i)$$

where $\sigma_x, \sigma_y, \sigma_z$ are the Pauli matrices and

$$Q(i) = \langle HF|\sum_\sigma c^\dagger_{i\sigma}c_{i\sigma}|HF\rangle = \sum_{p=1}^{N}\left[|\phi_p(i,\uparrow)|^2 + |\phi_p(i,\downarrow)|^2\right]$$

is the total number of electrons at site i, in the HF ground-state $|HF\rangle = \prod_{p=1}^N a^\dagger_p|0\rangle$. Similarly, $S_z(i) = \langle HF|\sum_\sigma \sigma/2c^\dagger_{i\sigma}c_{i\sigma}|HF\rangle$, and $S_+(i) = S_x(i) + iS_y(i) = \langle HF|c^\dagger_{i\uparrow}c_{i\downarrow}|HF\rangle$ are the expectation values for total spin (in units of $\hbar = 1$) at site i.

The self-consistent solution is a long-range order antiferromagnet, with $Q(i) = 1$ and $\vec{S}(i) = (-1)^i S\vec{e}_z$ (strictly speaking, you would have to verify this by comparing its energy against a ferro and a paramagnetic state – however, you showed in the previous problem that this Hamiltonian is equivalent to an AFM Heisenberg model, so this "guess" is justified). You can now solve the Hartree-Fock equations, with good quantum numbers $n \to (k, \sigma)$ (i.e., a spin and a quasi-momentum). Attention: since there are two different types of sites, you must divide the chain in $N/2$ unit cells of two-sites each. Count all the states to make sure you chose the appropriate Brillouin zone with the appropriate number of distinct states k, given by the cyclic boundary conditions.

Now that you have found $E_{k\sigma}$ and $\phi_{k\sigma}(i)$, check the self-consistency condition $Q(i) = 1$ for both even and odd sites. Similarly, show that the self-consistency condition for the magnitude of the staggered spin S is

$$S = \frac{US}{N} \sum_k \frac{1}{\sqrt{4t^2 \cos^2(ka) + (US)^2}}$$

where the sum is over the relevant Brillouin zone. In the limit $U >> t$, show that the self-consistent solution is $S = \frac{1}{2}(1 - 4t^2/U^2 + ...)$ (almost fully polarized).

4. **Fermionic coherent states**: consider a pair of fermionic operators $a, a^\dagger$ with the usual algebra $\{a, a^\dagger\} = 1, a^2 = (a^\dagger)^2 = 0$. We define a Grassman algebra with two generators ξ, ξ^* which satisfy: $\xi^2 = (\xi^*)^2 = 0, \xi\xi^* + \xi^*\xi = 0$ (i.e. any generator anticommutes with any other generator). We also require that ξ and ξ^* anticommute with a and $a^\dagger$, $a\xi + \xi a = 0$, etc.

a) show that the most general functions are of the form $f(\xi) = x_0 + c_1\xi; g(\xi, \xi^*) = c_0 + c_1\xi + c_2\xi^* + c_3\xi\xi^*$. Here the c's are complex variables.

b) by analogy with the boson coherent states, we define:

$$|\xi\rangle = e^{-\xi a^\dagger}|0\rangle$$

Using the rules given above, show that $a|\xi\rangle = \xi|\xi\rangle$. Also show that the overlap of two coherent states is: $\langle\xi|\xi'\rangle = e^{\xi^*\xi'}$ (again, similar to bosonic result).

c) we define the integration rules: $\int d\xi 1 = 0; \int d\xi\xi = 1$ and $\int d\xi^* 1 = 0; \int d\xi^*\xi^* = 1$. Note: the order in the integrant is important, the variable must be near the $d\xi$. Example: $\int d\xi\xi^*\xi = -\int d\xi\xi\xi^* = -\xi^*$ where we fist used anticommutation to bring ξ near $d\xi$, and then used the second rule. Also, $\int d\xi\xi^* = 0$ (first rule). We also have $\int d\xi \int d\xi^* = -\int d\xi^* \int d\xi$ (anticommutation again).

We can now define a δ function: $\delta(\xi, \xi') = \int d\eta e^{-\eta(\xi-\xi')}$. Show that (i) $\delta(\xi, \xi') = -(\xi - \xi')$ and (ii) for any $f(\xi)$, we have $\int d\xi'\delta(\xi, \xi')f(\xi') = f(\xi)$ –which is what we expect a δ-function to do.

d) Demonstrate the resolution of identity: $\int d\xi^* \int d\xi e^{-\xi^*\xi}|\xi\rangle\langle\xi| = 1$.

Note: there isn't anything difficult about all of this – just follow the rules blindly! Generalization to many fermionic states is hopefully more or less obvious.