Condensed Matter Physics

homework problems, set 1, fall 2015

deadline 20 November

Please structure your solutions carefully. All essential steps in your analysis and calculations should be made explicit. You are encouraged to study the problems together with your fellow students. However, you must take full responsibility for your own work, and, if you get questions about your solutions, you should be able to explain what you have done.

---

1. Consider the Hamiltonian for interacting electrons in a uniform distribution of positive charge,

$$\mathcal{H} = \sum_{\boldsymbol{k}} \mathcal{E}_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}} c_{\boldsymbol{k}} + \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}\neq 0} \frac{2\pi e^2}{V\boldsymbol{q}^2} c^\dagger_{\boldsymbol{k}-\boldsymbol{q}} c^\dagger_{\boldsymbol{k}'+\boldsymbol{q}} c_{\boldsymbol{k}'} c_{\boldsymbol{k}}.$$

Show that

$$[\sum_{\boldsymbol{k}} n_{\boldsymbol{k}}, \mathcal{H}] = 0.$$

Interpret the result!

Hint: First calculate the commutators between fermionic creation- and annihilation operators, using the fermionic anticommutation relations. Then obtain the commutators between the number operator and the creation- and annihilation operators. Using these, the problem can be solved fairly straightforwardly.

2. In my Friday lecture November 13 I briefly touch(ed) on a problem with the Hartree-Fock approximation: Something is amiss with the result for a particle-hole excitation,

$$\frac{dW}{dp} = \frac{\partial \mathcal{E}_{\boldsymbol{p}}}{\partial p} - \frac{\partial}{\partial p} \sum_{\boldsymbol{k}} \frac{4\pi e^2}{V\,|\boldsymbol{k}-\boldsymbol{p}|^2} \langle n_{\boldsymbol{k}} \rangle.$$

What exactly does this expression stand for? And why is there a problem with it?

Hint: Analyze the second term on the righ-hand side! Convert the sum to an integral, and pass to spherical coordinates. Do the integral. What do you find? Interpretation?

3. In the Hartree-Fock approximation the energy of interacting electrons in a uniform distribution of positive charge is given by

$$\mathcal{E}_{HF} = \mathcal{E}_0 \; - \sum_{\boldsymbol{k},\boldsymbol{k}' \text{ occupied}} \frac{2\pi e^2}{V\,|\boldsymbol{k}-\boldsymbol{k}'|^2},$$

where the summation in the exchange term, $\mathcal{E}_{exc}$, is taken only over states $\boldsymbol{k}$ and $\boldsymbol{k}'$ that are occupied and that have the same spin (reflecting the fact that the underlying Coulomb interaction is spin preserving). After some tedious calculus, having converted the sum in the exchange term $\mathcal{E}_{exc}$ to an integral, one finds that $\mathcal{E}_{exc}/N_e = -0.9 \times c_1 \times (N_e/V)^{1/3}$, where N_e is the number of electrons with the same spin, and where c_1 is a dimensionful constant. The kinetic term, $\mathcal{E}_0$, is more easy to calculate and one finds that $\mathcal{E}_0/N_e = 2.2 \times c_2 \times (N_e/V)^{2/3}$, where c_2 is another dimensionful constant taking roughly the same numerical value as c_1. It follows that Hartree-Fock theory predicts a phase transition into a magnetically ordered state where all electron spins point in the same direction. At what density of electrons would this happen? Does it really happen, or is it an artifact of the Hartree-Fock approximation?

Hint: There is not much to calculate here. This problem is more intended to illustrate a feature of Hartree-Fock theory. To answer the last question, "Does it really happen?", you may wish to do some literature search.