HomeWork 4

Reminder : the occupation number of a fermion at energy ε is given by the Fermi-Dirac distribution :

$$n(\varepsilon_k) = \frac{1}{e^{(\varepsilon_k - \mu)/T} + 1}$$

where μ is the chemical potential, T the temperature.

1 Appetizer : static structure factor

Calculate the static structure factor for non-interacting fermions

$$S^0(q) = \frac{1}{N}\langle\phi_0|\hat{n}_q \hat{n}_{-q}|\phi_0\rangle$$

where $\hat{n}_q = \sum_{k,\sigma} c^\dagger_{k\sigma} c_{k+q\sigma}$ is the particle density operator in the momentum representation and $|\phi_0\rangle$ is the Fermi sea. As usual, take the continuum limit $\sum_{k\sigma} = 2V \int d^3k/(2\pi)^3$ and calculate $S^0(q)$ explicitly.
Hint : Consider the cases $q = 0$ and $q \neq 0$ separately.

2 Modification of electron energy levels due to the Coulomb interaction

We consider a system of electrons interacting via the Coulomb repulsion. Thus, the Hamiltonian is a sum of a kinetic or free term, and a Coulomb term. (cf Homework 1)

$$H = H_0 + H_{Coulomb}$$

with

$$H_0 = \sum_{k\sigma} \frac{(\hbar k)^2}{2m} c^\dagger_{k\sigma} c_{k\sigma} = \sum_{k\sigma} \varepsilon_0(k) c^\dagger_{k\sigma} c_{k\sigma}$$

and

$$H_{Coulomb} = \frac{1}{2V} \sum_{q,p,k',\sigma,\sigma'} \frac{4\pi}{q^2} c^\dagger_{p+q,\sigma} c^\dagger_{k'-q,\sigma'} c_{k'\sigma'} c_{p\sigma}$$

The goal of this exercise is to calculate the modification of the electron energy levels due to the Coulomb interaction. To do so, we will work within the framework of the Hartree-Fock approximation.

2.1 First, we consider only H_0. Write the equation of motion for the operator $c_{k\sigma}(t)$ in the absence of Coulomb interaction.

2.2 Using the preceding result, derive an equation for the time evolution of the Green's function (already introduced in Homework 3) :

$$G_{k\sigma}(t) = \langle\psi_0|c_{k\sigma}(t) c^\dagger_{k\sigma}(0)|\psi_0\rangle$$

Solve this equation.

2.3 Now on, we include $H_{Coulomb}$. Write down the new equation of motion satisfied by $c_{k\sigma}$.

2.4 Prove that the Green's function now satisfies

$$\frac{d}{dt}G_{k\sigma}(t) = -\frac{i}{\hbar}\left(\varepsilon_0(k)G_{k\sigma}(t) - \frac{1}{V}\sum_{p,q\neq 0,\sigma'}\frac{4\pi e^2}{q^2}\left\langle c^\dagger_{p+q,\sigma'}c_{k+q,\sigma}c_{p\sigma'}c^\dagger_{k\sigma}(-t)\right\rangle\right),$$

where in the last term we have carried out a translation in time by $-t$ and have written $c_{k\sigma} \equiv c_{k\sigma}(0)$ etc.

2.5 On the right hand side of the equation for $G_{k\sigma}$ now appears a higher-order correlator. The Hartree-Fock approximation consists in factorizing this 4-body term into a product of two 2-body correlators as follows :

$$\left\langle c^\dagger_{p+q,\sigma'}c_{k+q,\sigma}c_{p\sigma'}c^\dagger_{k\sigma}(-t)\right\rangle = \left\langle c^\dagger_{p+q,\sigma'}c_{k+q,\sigma}\right\rangle\left\langle c_{p\sigma'}c^\dagger_{k\sigma}(-t)\right\rangle = \delta_{\sigma\sigma'}\delta_{pk}\left\langle c^\dagger_{p+q,\sigma'}c_{p+q,\sigma'}\right\rangle\left\langle c_{k\sigma}c^\dagger_{k\sigma}(-t)\right\rangle.$$

Using the Hartree-Fock approach, rewrite the equation obtained in **2.4** and prove that the dispersion relation of an electron has now the form :

$$\varepsilon(k) = \frac{\hbar^2k^2}{2m} - \frac{1}{V}\sum_{k'}\frac{4\pi e^2}{|k-k'|^2}n_{k'\sigma}.$$

2.6 The second term in $\varepsilon(k)$ leads to a deviation form the "free" energy. Evaluate this deviation $\Delta\varepsilon(k)$ for $T = 0$, by explicitly carrying the sum over k' (take the continuum limit). *Help* : the result should be expressed with the function

$$F(x) = \frac{1}{2} - \frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|$$

where $x = k/k_F$, k_F being the Fermi cutoff for the momentum.
Plot $\Delta\varepsilon(k)$ and comment.