Exercises FYS-KJM4480, Fall semester 2009

Exercises week 43, October 19-23 2009

Exercise 15

The electron gas model allows closed form solutions for quantities like the single-particle Hartree-Fock energy. The latter quantity is given by the following expression

$$\varepsilon_k^{HF} = \frac{\hbar^2 k^2}{2m} - \frac{e^2}{V^2} \sum_{k' \leq k_F} \int d\vec{r} e^{i(\vec{k'}-\vec{k})\vec{r}} \int d\vec{r'} \frac{e^{i(\vec{k}-\vec{k'})\vec{r'}}}{|\vec{r}-\vec{r'}|}$$

a) Show that

$$\varepsilon_k^{HF} = \frac{\hbar^2 k^2}{2m} - \frac{e^2 k_F}{2\pi}\left[2 + \frac{k_F^2 - k^2}{k k_F} ln \left|\frac{k+k_F}{k-k_F}\right|\right]$$

(Hint: Introduce the convergence factor $e^{-\mu|\vec{r}-\vec{r'}|}$ in the potential and use $\sum_{\vec{k}} \rightarrow \frac{V}{(2\pi)^3}\int d\vec{k}$)
b) Rewrite the above result as a function of the density

$$n = \frac{k_F^3}{3\pi^2} = \frac{3}{4\pi r_s^3},$$

where $n = N/V$, N being the number of particles, and r_s is the radius of a sphere which represents the volum per conducting electron. It can be convenient to use the Bohr radius $a_0 = \hbar^2/e^2 m$.

For most metals we have a relation $r_s/a_0 \sim 2-6$.

Make a plot of the free electron energy and the Hartree-Fock energy and discuss the behavior around the Fermi surface. Extract also the Hartree-Fock band width $\Delta\varepsilon^{HF}$ defined as

$$\Delta\varepsilon^{HF} = \varepsilon_{k_F}^{HF} - \varepsilon_0^{HF}.$$

Compare this results with the corresponding one for a free electron and comment your results. How large is the contribution due to the exchange term in the Hartree-Fock equation?
c) We will now define a quantity called the effective mass. For $|\vec{k}|$ near k_F, we can Taylor expand the Hartree-Fock energy as

$$\varepsilon_k^{HF} = \varepsilon_{k_F}^{HF} + \left(\frac{\partial \varepsilon_k^{HF}}{\partial k}\right)_{k_F} (k - k_F) + \dots$$

If we compare the latter with the corresponding expressiyon for the non-interacting system

$$\varepsilon_k^{(0)} = \frac{\hbar^2 k_F^2}{2m} + \frac{\hbar^2 k_F}{m}(k-k_F) + \dots,$$

we can define the so-called effective Hartree-Fock mass as

$$m_{HF}^* \equiv \hbar^2 k_F \left(\frac{\partial \varepsilon_k^{HF}}{\partial k}\right)_{k_F}^{-1}$$

Compute m_{HF}^* and comment your results after you have done point d).
d) Show that the level density (the number of single-electron states per unit energy) can be written as

$$n(\varepsilon) = \frac{V k^2}{2\pi^2}\left(\frac{\partial \varepsilon}{\partial k}\right)^{-1}$$

Calculate $n(\varepsilon_F^{HF})$ and comment the results from c) and d).