Condensed Matter Physics II. – A.A. 2009-20010, April 26 2010

(*time 3 hours*)

Solve the following two exercises, each has a maximum score of 18 for a total of 36. A score between 33 e 36 corresponds to 30 cum laude, between 30 e 32 is renormalized to 30 (the maximum official score, without laude).

NOTE:

- Give all details which help in understanding the proposed solution. Answers which only contain the final result or not enough detail will be judged insufficient and discarded;
- If you are requested to give evaluation/estimates, do so using 3 significant figures.

Exercise 1: *1D electron gas in an external potential: LDA*

Consider non interacting electrons (at $T = 0$), moving in 1 dimension. Use atomic units ($\hbar = e = m_e = 1$) throughout the exercise.

1. Consider first the homogeneous electron gas (in 1D !) and give the relation between the density n and the Fermi wavevector for spin unpolarized electrons ($n_\uparrow = n_\downarrow = n/2$).
2. Knowing that in 1D for the homogeneous electron gas the kinetic energy per particle is $t = T/N = \epsilon_F/3$, write (for an inhomogeneous electron gas) the total kinetic energy functional $T[n]$ in the local density approximation (LDA).
3. Consider now the electron gas under the action of an external potential, so that the total energy functional $E[n] = T[n] + \int dx\, n(x)v(x)$ and write the extremum condition obeyed by this functional (at fixed external potential). Beware: the variation must be made with the constrain that $\int dx\, n(x) = N$. This requires consideration of a Lagrange multiplier that we shall denote by μ and call *chemical potential.*
4. Solve for $n(x)$ as function of $v(x)$ and μ
5. if $v(x) = V_0 sin^2(x)$, with $V_0 = \pi/4$, what is the condition that μ must satisfy, in order to get physical values for $n(x)$? Obtain the simplest possible expression for $n(x)$ when $\mu = \pi/4$.
6. Give a sketch of $n(x)$ in the particular case considered above ($V_0 = \mu = \pi/4$) for $-\pi \leq x \leq \pi$.

Exercise 2: *Conductivity in a doped semiconductor: metal-insulator transition.*

Consider the crystalline semiconductor InSb, with a direct gap ($E_g \approx 0.2eV$), an effective mass $m_c = 0.015m_e$ in the conduction band and two valence bands with effective masses $m_v = 0.2m_e$ e $m_v = 0.015m_e$. In the following consider only the heavy holes. (Why, by the way?). The dielectric constant of InSb is $\epsilon = 17.88$.

Let's dope the semiconductor with donors and describe the states of the extra electrons using the hydrogenoid model.

1. Calculate the binding energy of the extra electrons on the donors E_d (in eV), with respect to the bottom of the conduction band.

2. Calculate the effective Bohr radius a_B^* (in $\mathring{A}$) of such electrons and say if it is compatible with the assumed hydrogenoid approximation.

3. Let's assume that when the average donor-donor distance becomes comparable to a_B^* (which measure the size of the electron orbit in the ground state) the extra electron unbind and end up in the conduction band due to screening effects. At which critical donor density n_{cr} does it happens? Give n_{cr} in cm^{-3}.
[It is suggested to write the average donor density as $n_d = [(4\pi/3)a^3]^{-1}$ and to regard a as measure of the donor-donor distance.]

4. Estimate the intrinsic density (n_i, in cm^{-3}) at $T = 100K^o$ in the semiconductor without dopants, using the data given at the beginning of this exercise.

5. Comparing the carrier density obtained at the point 4 and 5 above say if at $T = 100K^o$ and for $n_d > n_{cr}$ the doped semiconductor is in the extrinsic or intrinsic regime.

6. At $T = 0$ and for $n_d > n_{cr}$, the doped semiconductor would be a an insulator or a metal and why?