Condensed Matter Physics II. – A.A. 2014-2015, April 30 2015

(*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: *HF-LDA for electrons in 2D in and external potential*

Consider electrons in 2 dimensions under the action of an external potential $v(r)$. We shall approximate the "internal energy of the electron system using the LDA and the HF approximations. To this end we recall that the energy per particle of an unpolarized electron system on an homogeneous charge background, according to Hartree-Fock, is in 2D

$$\epsilon = \frac{1}{2}\frac{\hbar^2}{2m}k_F^2 - \frac{4e^2}{3\pi}k_F,$$

where k_F is the Fermi wavevector for the system.

1. Use the expression of k_F in terms of the areal density ρ to give $\epsilon(\rho)$ **in atomic units** ($\hbar = 1$, $m = 1$, $e^2 = 1$).
2. Use the $\epsilon(\rho)$ obtained above to approximate the internal energy $E_I[\rho]$ of the inhomogeneneous electron gas in the LDA approximation, i.e., write down $E_I^{LDA}[\rho]$.
3. Consider now the electron gas under the action of an external potential $v(r)$ and write down the total energy functional by adding to $E_I^{LDA}[\rho]$ found above the energy of interaction between the electrons and the external potential. Derive the extremum condition that the equilibrium (ground state) density must satisfy.
4. Specialize the extremum condition to the case $\mu = \alpha^2(2/\pi^2)$, $v(r) = r^2(2/\pi^2)$, setting $\rho_0 = 2/\pi^3$, to get an equation for $\rho(r)/\rho_0$. Here μ denotes the chemical potential (i.e., the Lagrange multiplier introduced above) and $\alpha > 0$.
5. Solve the extremum condition for the particular case given above to obtain the density $\rho(r)/\rho_0$. Since you have to choose between three possible solutions (the two solutions of a quadratic equation and the solution $\rho(r) = 0$), keep in mind that (i) $\rho(r) \geq 0$, (ii) $\rho(r)$ must be continuous, (iii) you want a solution over all space, though you can chose different solutions in different ranges, provided you satisfy continuity.
6. Provide a qualitative sketch of $\rho(r)/\rho_0$ for $\alpha = 10$, over the entire r-axis, i.e., $0 \leq r \leq \infty$.

Exercise 2: *Doped semiconductor*

Note: In this exercise the numerical estimates must be given with 5 significant digits.

Consider a semiconductor in the intrinsic regime with an energy gap gap $E_g = 1.1200eV$. It is known from cyclotron resonance experiments at $B = 1000$ gauss that electrons at the top of the valence band have $\omega_c = 3.59 \times 10^{10}$ cycles and electrons at the bottom of the conduction band $\omega_c = 5.18 \times 10^{10}$ cycles. It is also known that the photoabsorption threshold of the semiconductor doped only with donors is at 0.0338 eV. Both the conduction and valence bands have a spherical dispersion.

1. Evaluate the effective masses at the bottom of the conduction band and the the top of the valence band, in units of m_e.
2. What is the value (in eV) of the binding energy of the donor level?
3. What is the value of the dielectric constant of the semiconductor?
4. Compute the effective Bohr radius a_B^* of the donor level (in units of a_B).
5. Is the hydrogenic approximation reasonable for donors? Motivate your answer.
6. At which energy photoabsorption would begin (i) when only acceptors are present and (ii) when acceptors and donors are present and $N_d > N_a$?