Condensed Matter Physics II. – A.A. 2018-2019, 10 maggio, 2019

(*time 3 hours*)

Solve the following two exercises.

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: *LDA (with exchange) for the electron gas*

1. Consider the energy per particle of the electron gas (eq. 17.23, Aschcrogt & Mermin), express it in terms of the density $\rho = N/V$, name it $\epsilon(\rho)$, and use atomic units, $\hbar = e = m = 1$. I suggest that you define two constants for the coefficients of the two density powers.
2. Write the internal energy functional (kinetic + exchange energies only!) .
3. Using the result above, write the full energy functional (kinetic + exchange energies + interaction with external potential $v(\mathbf{r})$) and impose the extremum condition.
4. Use the extremum condition to obtain an expression for $\rho(\mathbf{r})$. As you should have got a quadratic equation you should have two solutions.
5. Demonstrate that if the second functional derivative with respect to $\rho(\mathbf{r})$ of the energy funcional has the form $g(\rho(\mathbf{r}))\delta(\mathbf{r} - \mathbf{r}')$ a necessary condition for a minimum is that $g(\rho(\mathbf{r})) > 0$.
6. Calculate the second functional derivative with respect to $\rho(\mathbf{r})$ of the energy funcional and use it to select the solution that correspond to a minimum.
7. If $v(\mathbf{r}) = -V_0\theta(R - r)$, what is the condition on μ in order to get a finite number of particles in the potential well?

Exercise 2: *Doped semiconductor*

Consider a semiconductor in the intrinsic regime with an energy gap gap $E_g = 1.43eV$. It is known from cyclotron resonance experiments at $B = 1$ tesla that electrons at the top of the valence band have $\omega_c = 3.52 \times 10^{11}$ cycles and electrons at the bottom of the conduction band $\omega_c = 2.67 \times 10^{12}$ cycles. It is also known that the photoabsorption threshold of the semiconductor at very low temperature and doped only with donors is at 5.07×10^{-3} 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 very low temperature, at which energy photoabsorption would begin (i) when only acceptors are present and (ii) when acceptors and donors are present and $N_d > N_a$?