Condensed Matter Physics II. – A.A. 2019-2020, April 30 2020

(*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.

Esercizio 1: *LDA for Fermions in graphene*

Consider N non-interacting spin 1/2 Fermions with an energy dispersion mimicking that of electrons in a single graphene sheet doped with electrons. Thus the Fermions move in 2D (on the surface A) with a single-particle energy dispersion $\epsilon_{\sigma,\tau}(\mathbf{p}) = v^*|\mathbf{p}|$, for given spin projection ($\sigma = \pm 1$) and valley index ($\tau = \pm 1$), with $v^* > 0$ a characteristic velocity. Consider periodic boundary conditions (PBC). Restrict to the spin and valley unpolarized state, i.e., equal populations for up and down spin projections and the two valleys.

1. Calculate the Fermi momentunm p_F and express the Fermi energy E_F in terms of the areal number density $n = N/A$.
2. Calculate the ground state energy (total energy) of such system, and from it the energy per Fermion $\varepsilon(n)$.
3. Consider now the same system of Fermions in an external potential $v(\mathbf{r})$ and write the totale energy (kinetic + interaction with the external potential) resorting to the Local Density Approximation (LDA) for the kinetic energy.
4. Obtain the equilibrium density (from the minimum energy principle).
5. Calculate the linear response function defined by

$$\chi_0(\mathbf{r}, \mathbf{r}') = \left.\frac{\delta n(\mathbf{r})}{\delta v(\mathbf{r}')}\right|_{v=0}.$$

   You should find $\chi_0(\mathbf{r}, \mathbf{r}') = \chi_0(|\mathbf{r} - \mathbf{r}'|)$.

6. Calculate the Fourier transform of the response function

$$\chi(q) = \int d\mathbf{r}\, \chi(r) e^{i\mathbf{q}\cdot\mathbf{r}}.$$

   This result should be exact in the limit of long wavelengths.

Esercizio 2: Chemical potential in a donor doped semiconductor

Consider a semiconductor withy direct gap (E_g) and non degenerate conduction and valence bands, doped with monovalent donors with density N_d. The binding energy of one electron on the dono center is $\epsilon_b > 0$ so that the corresponding electron energy level is with obvious notation $\epsilon_d = \epsilon_c - \epsilon_b$. The donor binding is very shallow in comparison with the energy gap, $\epsilon_b \ll E_g$

1. Say what are at $T = 0$ the following occupation numbers:p_v, n_d, n_c.
2. Locate the position of the chemical potential μ when $T \to 0$.
3. For $K_B T \lesssim \epsilon_b$ assuming that for such low temperature μ maintains the value found above and the non-degenerate assumption for $n_c(T)$ holds copy the relevant expression of $n_c(T)$ from the Ashcroft and Mermin (AS).
4. When temperature is raised one expects that electrons from donors are the first to migrate to the conduction band, given the much smaller amount off energy needed compared with electrons in the valence band, as $\epsilon_b \ll E_g$. Assuming that as T is raised from 0 initially μ does not move appreciably, use the $n_c(T)$ copie above to get the temperature T^* at which $n_c(T^*) = N_d$. In doing so, as T appears both in an exponential and in $N_c(T)$, solve for the T^* in the exponential, in terms of the rest, including $N_c(T^*)$. In other words you get an implicitamente equation for T^*.
5. At temperature $K_B T \lesssim \epsilon_b$ what is the expression of $p_v(T)/n_c(T)$ assuming $m_c = m_v$.
6. For temperature $T \gtrsim T^*$ the μ will start moving downward. As the donors will be completely ionized, start from eq. (28.35) of AS, specialized to the present case, to obtain μ in terms of μ_i, T, N_d, $n_i(T)$.