Condensed Matter Physics II. – A.A. 2023-2024, April 17, 2024

(*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: *Screening in a 2-dimensional electron gas at long wavelengths*

Consider electrons in 2D on a rigid uniform neutralizing charge background in the presence of a potential energy field $\Phi_{ext}(\mathbf{r})$ due to external charges. The energy functional for the system is::

$$E[\rho] = T_0[\rho] + U_{xc}[\rho] + \frac{e^2}{2}\int d\mathbf{r}\int d\mathbf{r}'\,\frac{\rho_Q(\mathbf{r})\rho_Q(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + \int d\mathbf{r}\rho_Q(\mathbf{r})\Phi_{ext}(\mathbf{r}),$$

where $\rho(\mathbf{r})$ is the electron density and $\rho_Q(\mathbf{r}) = \rho(\mathbf{r}) - \rho_b$, with ρ_b the density of background charges. Use the LDA approximation for the first two terms in the functional above, setting

$$E_{LDA}[\rho] = \int d\mathbf{r}\rho(\mathbf{r})\varepsilon(\rho(\mathbf{r})) + \frac{e^2}{2}\int d\mathbf{r}\int d\mathbf{r}'\,\frac{\rho_Q(\mathbf{r})\rho_Q(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + \int d\mathbf{r}\rho_Q(\mathbf{r})\Phi_{ext}(\mathbf{r}),$$

with $\varepsilon(\rho)$ the energy per particle of the homogeneous 2D electron gas, assumed known. This approximation should become accurate in the long wavelength limit.

1. Write the extremum condition for the above functional.
2. Rearrange the terms involving $\varepsilon(\rho(\mathbf{r})$ and $d\varepsilon(\rho)/\rho|_{\rho(\mathbf{r})}$ so that $\mu(\rho(\mathbf{r}))$ appears.
3. Obtain the Lagrange multiplier introduced in the point 1 above (say λ) when $\Phi_{ext}(\mathbf{r}) = 0$ (homogeneous electron gas).
4. For $\Phi_{ext}(\mathbf{r})$ small we expect $\rho_Q(\mathbf{r})$ to be much smaller than ρ_b and therefore linearize in $\rho_Q(\mathbf{r})$ the extremum condition.
5. Obtain the linear proper response, i.e. the response $\tilde{\chi}(q)$ to the total potential energy field $\Phi(\mathbf{q})$,
$$\tilde{\chi}(q) = \frac{\rho_Q(\mathbf{q})}{\Phi(\mathbf{q})}$$
6. Knowing the response $\tilde{\chi}(q)$ you can immediately write down the dielectric function $\epsilon(q)$. Beware: the Fourier transform of the electron-electron interaction appears explicitely in $\epsilon(q)$ and it is different for different dimensions. In 2D the Fourier transform of $1/r$ is $2\pi/q$.

Exercise 2: *Model semiconductor in the degenerate and intrinsic regime*

Let's consider a model semiconductor in the degenerate, intrinsic regime: in other words, we consider a semiconductor for which it is **not** possibile to assume neither $\epsilon_c - \mu \gg K_B T$ nor $\mu - \epsilon_v \gg K_B T$. Moreover, we assume that the impurity concentration is negligible (intrinsic regime).The semiconductor density of states, however, satisfies: $g_v(\epsilon^* - \epsilon) = g_c(\epsilon^* + \epsilon)$, with $\epsilon^* = (\epsilon_c + \epsilon_v)/2$.

1. Assuming that the maximum of the conduction band is at $\epsilon_c + 2\Delta$, provide a qualitative sketch of $g_c(\epsilon)$, with the correct qualititative behavior at ϵ_c and $\epsilon_c + 2\Delta$: please indicate explicitely such qualitative behaviors. Here and in the following it is suggested to take ϵ^* as zero of energy.

2. Give a qualitative sketch (on the same graph) of $g_v(\epsilon)$ and $g_c(\epsilon)$.

3. Write down the condition that determines the chemical potential, keeping in mind that the Fermi distribution cannot be approximated in any way, due to the degenerate regime: in othe words, impose $n_c(T, \mu) = p_v(T, \mu)$, with obvious notation. It is suggested that you rearrange the two integrals providing the carrier concentrations in a form that allows the determination of μ by inspection. [*Note, you do not need to perfom any integral!*].

4. Consider now a density of states $g_c(\epsilon) = A\sqrt{(\epsilon - \epsilon_c)(2\Delta - \epsilon + \epsilon_c)}$. Determine A as function of ρ_L and Δ, knowing that the system is a Bravais with one atom/site, that the density of states results from just one band and that ρ_L is the density of lattice sites in space.

5. Express the effective mass at the bottom of the conduction band in terms of ρ_L and Δ.

6. Knowing that $\rho_L = 5.00 \times 10^{22} cm^{-3}$and $\Delta = 27.7eV$ evaluate m_c/m_e with 3 significant figures.