WS14/15 Condensed Matter Physics I
Exercise 6. Semiconductors.

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Notice*: In solving the proposed exercises clearly motivate the passages to reach the result. The use of clear and compact notation is greatly encouraged, as well as the systematic use of dimensional checks of the expressions and results. When you are asked to "evaluate" something this means to provide a numerical evaluation of the expression. In this case, at times, it might be necessary to indicate a parameter whose explicit numerical value is not provided, i.e. $\omega_c = 1.76\, H$ (Gauss) Hertz. Otherwise specified, all the evaluations are to be given with 3 significant figures.*

6.1   conductivity from impurities   (10 pts)

Let us consider the semiconductor GaAs (gallium arsenide). It is a direct gap semiconductor ($E_g \simeq 1.52\, eV$ at room temperature; disregard its temperature dependence). The conduction band effective mass is $m_c = 0.068\, m_e$ and the valence band $m_v = 0.41\, m_e$. The dielectric constant is $\epsilon = 14.6$.

Let us assume to dope the semiconductor with donors and suppose to describe the status of the excess electrons with a *hydrogenoid* model.

1. Calculate the binding energy E_d (in eV) of the excess electrons with respect to the conduction band bottom.
    [The binding energy of the excess electron is the renormalized hydrogenoid ground state [Ashcroft Eq. 28.29]

    $$\mathcal{E} = \frac{m_c}{m}\frac{Ry}{\epsilon^2} = \frac{0.068}{14.6^2}\,13.6\text{ eV} = 4.34\text{ meV}.$$

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2. Calculate the effective Bohr radius a_B^* (in Å) of those electrons, assuming that each of them is in the fundamental hydrogenoid energy level. Is the value obtained compatible with the hydrogenoid model used?
    [The effective Bohr radius [Ashcroft Eq. 28.28] is

$$a_B^* = \frac{m_c}{m^*} \epsilon a_0 = \frac{14.6}{0.068} \, 0.53 \, \text{Å} = 114 \, \text{Å}$$

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3. Assume that when the average distance between donor centers becomes comparable to a_B^* the electron screen each other, becoming nearly-free electrons and being promoted to the conduction band. Evaluate the value n_{cr} of the donor (and electron) density $in \; cm^{-3}$.

   [The critical donor center is $n_{cr} = (a_B^*)^{-3} = 6.79 \times 10^{17} \text{cm}^{-3}$]

4. Estimate the carrier density (electron and holes; $n_c + p_v \; in \; cm^{-3}$) of the undoped semiconductor at the temperature of T=100 K by using the data given in the preamble.

   [In the intrinsic case $n_c = p_v = n_i$, We can therefore apply the Equation 28.20 of the Ashcroft:

   $$n_i(T) = 2.5 \left(\frac{m_c}{m}\right)^{3/4} \left(\frac{m_v}{m}\right)^{3/4} \left(\frac{T}{300 \; K}\right)^{3/2} e^{-E_g/2k_BT} \times 10^{19} \; cm^{-3} =$$

   For T=10 K we have

   $$n_c + p_v = 2n_i(T = 100 \; K) = 1.35 \times 10^{-21} \; cm^{-3}.$$

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5. By comparing the densities obtained at points 3 and 4 tell estimate if at T=100 K and for $n_d > n_{cr}$ the doped semiconductor is in the extrinsic (doping dominated) or intrinsic regime.

   [The semiconductor is in the extrinsic regime.]

6. At T=0 and for a donor density $n_d > n_{cr}$, is the GaAs an insulator, a semiconductor or a metal? Why?

   [At T=0 the conduction band is still populated by the self screened donors. Therefore the material is a metal.]

6.2   Current in a Landau Level   (10 pts)

Let us consider 2D free electron in a magnetic field B. In the Landau Gauge the vector potential is $\mathbf{A} = (0, Bx)$. The Hamiltonian is

$$H = \frac{\hbar^2}{2m} \left[-\frac{\partial^2}{\partial x^2} + \left(-i\frac{\partial}{\partial y} + \frac{x}{\ell^2}\right)^2 \right],$$

Where $\ell = \sqrt{\hbar c/eB}$. Note that the component of the velocity operator are $v_x = -\frac{i\hbar}{m}\frac{\partial}{\partial x}$ and $v_y = \frac{\hbar}{m}\left(-i\frac{\partial}{\partial y} + \frac{x}{\ell^2}\right)$. The levels for this Hamiltonian are discreet and the eigenfunctions at the lowest level can be chosen as

$$\psi_k(x, y) = e^{iky}\chi(x + \ell^2 k), \qquad \chi(x) = \left(\frac{1}{\pi\ell^2}\right)^{1/4} e^{-x^2/2\ell^2},$$

where k is a real number. The $\chi(x)$ is normalized over $(-\infty, \infty)$.

1. Calculate the current on the generic state k, disregarding the normalization:

$$j_x(x, y) \propto \psi_k^*(x, y)v_x\psi_k(x, y) + c.c. \quad \text{and} \quad j_y(x, y) \propto \psi_k^*(x, y)v_y\psi_k(x, y) + c.c.$$

[For the x direction we have

$$j_x(x, y) \propto \psi_k^*(x, y)v_x\psi_k(x, y) + c.c. = \left(-\frac{i\hbar}{m}\right)\chi^2(x + \ell^2 k)\frac{x + \ell^2 k}{\ell^2} + c.c. = 0$$

As expected, the current along the x direction is vanishing. For the y direction we have

$$j_y(x, y) \propto \frac{2\hbar}{m}\chi^2(x + \ell^2 k)\left[k + \frac{x}{\ell^2}\right].$$

The current along the y direction depends only on the x direction.]

2. Impose now periodic boundary conditions along y: $\psi_k(x, y) = \psi_k(x, y + L)$. This allows only some values of k to be admissible. Which ones? Write the generic wavefunction normalized over the appropriate cell.

[The admissible values are found by applying the definition of the periodic wavefunction:

$$e^{iky} = e^{ik(y+L)} \Rightarrow k_n = \frac{2\pi n}{L}$$

The wavefunciton has to be normalized on the cell of length L: therefore

$$\psi_n(x, y) = \frac{1}{\sqrt{L}}e^{ik_n y}\chi(x + \ell^2 k_n).$$

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3. Let us now consider non interacting electrons occupying all the allowed k's. Obtain the density

$$n(x, y) = \sum_{k\ allowed} |\psi_k(x, y)|^2.$$

How this density depends from the y direction? Is the density n periodic along x? with which period?

[The density is given by

$$n(x, y) = \sum_{k\ allowed} |\psi_k(x, y)|^2 = \frac{1}{L}\sum_n \chi^2(x + \ell^2 k_n)$$

$$= \frac{1}{L}\left(\frac{1}{\pi\ell^2}\right)^{1/2}\sum_n e^{-(x+2\pi n\ell^2/L)^2/\ell^2}$$

We can see that the density does not depend on the y direction, consistent with the fact that the current along y depends only on the x variable. On the other side, the current is a sum of Gaussians, each translated by a fixed length. This induces a period of $2\pi\ell^2/L = hc/eLB$.]

6.3   Degenerate semiconductor   (10 pts)

Consider a semiconductor for which the non-degeneracy condition is not verified. In other words you **cannot** assume $\epsilon_c - \mu \gg K_B T$ and $\mu - \epsilon_v \gg K_B T$. However, for this semiconductor the following relation

$$g_v(\epsilon) = g_c(-[\epsilon - E_0] + E_0)$$

holds. Here $g_v(\epsilon)$ and $g_c(\epsilon)$ are the DOS of the valence and conduction bands and $2E_0 = \epsilon_c + \epsilon_v$. Moreover it is possible to neglect the impurity (intrinsic regime).

1. Assume that the top of the conduction band is at the energy $\epsilon_c + 2\Delta$. Draw a qualitative drawing of the density of states $g_c(\epsilon)$, paying attention to its behavior at the two band extrema. In particular specify the qualitative behavior of the DOS at those points.
2. By making use of the above-written relation, draw on the same graph $g_c(\epsilon)$ and $g_v(\epsilon)$.
3. Write the condition that determines the chemical potential and, by rearranging in a simple way one of the integrals, determine the chemical potential μ at every temperature. *[Note: no explicit integration is needed! Moreover, put the energy zero at the half of the gap, in such a way that $2E_0 = \epsilon_c + \epsilon_v = 0$.]*

[The condition that determines the chemical potential for an intrinsic semiconductor is $n - p = 0$, I.e. the number of electrons is equal to the number of holes. The electron and hole density is given by [Ashcroft eq. 28.9]:

$$n = \int_{\epsilon_c}^{+\infty} d\epsilon \, \frac{g_c(\epsilon)}{e^{\beta(\epsilon-\mu)} + 1}, \qquad p = \int_{-\infty}^{\epsilon_v} d\epsilon \, \frac{g_v(\epsilon)}{e^{\beta(\mu-\epsilon)} + 1}$$

By putting the zero of the energy at the half of the gap we have $\epsilon_c = -\epsilon_v = E_0/2$; moreover with this choice we have

$$g_v(\epsilon) = g_c(-\epsilon)$$

Therefore

$$n - p = \int_{E_0/2}^{+\infty} d\epsilon \, \frac{g_c(\epsilon)}{e^{\beta(\epsilon-\mu)} + 1} - \int_{-\infty}^{-E_0/2} d\epsilon \, \frac{g_c(-\epsilon)}{e^{\beta(\mu-\epsilon)} + 1} = 0.$$

we can change the variable in the second integral $\epsilon \rightarrow -\epsilon$; in this case the integration limits become the same and we get:]

$$n - p = \int_{E_0/2}^{+\infty} d\epsilon \, g_c(\epsilon) \left[\frac{1}{e^{\beta(\epsilon - \mu)} + 1} - \frac{1}{e^{\beta(\mu + \epsilon)} + 1} \right]$$

$$= \sinh \beta\mu \int_{E_0/2}^{+\infty} d\epsilon \, g_c(\epsilon) \frac{1}{\cosh \beta\epsilon + \cosh \beta\mu} = 0.$$

The integrand is definite positive over the integration limit, therefore it cannot vanish. The only way that the equation is satisfied is $\sinh \beta\mu = 0$, i.e. $\mu = 0$ for any T. This means the chemical potential remains at the middle of the gap. This is also logic since the conduction and valence band DOS are the one the mirror image of the other .
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4. Consider now a density of states of the form $g_c(\epsilon) = A\sqrt{(\epsilon - \epsilon_c)(2\Delta - \epsilon + \epsilon_c)}$. Determine the constant A in terms of the density of lattice sites n_L and Δ.

[The normalization condition on the density of states is [Ashcroft 8.58].

$$\int_{-\infty}^{+\infty} d\epsilon g_c(\epsilon) = 2n_L$$

Therefore, by taking into account the bandwidth, we have

$$A \int_{\epsilon_c}^{\epsilon_c + 2\Delta} d\epsilon \sqrt{(\epsilon - \epsilon_c)(2\Delta - \epsilon + \epsilon_c)} = 2n_L$$

By performing the change of variable $u = \epsilon - \Delta - \epsilon_c$ to put the zero at the band centre. We therefore get the symmetric integral

$$A \int_{-\Delta}^{\Delta} du \sqrt{\Delta^2 - u^2} = \Delta A \int_{-\Delta}^{\Delta} du \sqrt{1 - \frac{u^2}{\Delta^2}} = \Delta^2 A \int_{-1}^{1} dt \sqrt{1 - t^2}$$

$$= \Delta^2 A \arcsin 1 = \frac{\pi \Delta^2 A}{2} = 2n_L.$$

By making use of the note. Therefore we have $A = 4n_L / \pi \Delta^2$. Of course the normalization does not depend on the conduction band position but only on the bandwidth.]

5. Express the effective mass at the bottom of the conduction band in terms of n_L and Δ. Knowing that $n_L = 5.00 \times 10^{22} \, cm^{-3}$ and that $\Delta = 27.7$ eV evaluate the ratio m_c / m_e.

[Around the conduction band bottom ($\epsilon \simeq \epsilon_c$) we have

$$g_c(\epsilon) \simeq \frac{2^{5/2} n_L}{\pi \Delta^{3/2}} \sqrt{\epsilon - \epsilon_c}$$

By comparing this result to the DOS of a free electron dispersion [Ashcroft eq. 2.61]

$g_{fel}(\epsilon) \simeq \frac{\sqrt{2} m_{eff}^{3/2}}{\pi^2 \hbar^3} \sqrt{\epsilon - \epsilon_c}$ we get the effective mass in terms of the density and bandwidth:

$$m_{eff} = \frac{\hbar^2}{\Delta}(4\pi n_L)^{2/3}$$

In terms of Hartree atomic units ($e = \hbar = m_e = 1$) we have $\Delta = 1.02$ Hartree, $n_L = 7.44 \times 10^{-3} \, a_0^{-3}$. Therefore we obtain a value of $m_{eff} = 0.202 \, m_e$.]

Note: $\int dx\sqrt{1 - x^2} = \left[x\sqrt{1 - x^2} + \arcsin x\right]/2.$