



WS16/17 Condensed Matter Physics I
Exercise 5. 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.

5.1 Two-charge-carrier Drude Model (10 pts)

In treating the Hall problem in the presence of a magnetic field H along the z axis, it is useful to resort to the tensor formalism to link the components of the in-plane electric field and current:

$$\mathbf{E} = \hat{\rho} \mathbf{j}$$

where the resistivity tensor $\hat{\rho}$ depends on the longitudinal resistivity ρ and the Hall resistivity R_H :

$$\hat{\rho} = \begin{pmatrix} \rho & -R_H H \\ R_H H & \rho \end{pmatrix}.$$

For a single carrier in the Drude model we have $\rho = \frac{1}{\sigma} = \frac{1}{ne^2\mu}$ and $R_H = \frac{1}{nec}$.

Consider now a system with two types of charge carriers in the Drude model. The two carriers have the same density (n) and opposite charge (e and $-e$), and their masses and relaxation rates are m_1, m_2 and τ_1, τ_2 , respectively. (You may want to use the mobility, $\mu = \tau/m$, instead of τ and m .)

1. Introduce the two resistivity tensors $\hat{\rho}_1$ and $\hat{\rho}_2$ write down the equation linking the electric field and the two carrier currents \mathbf{j}_1 and \mathbf{j}_2 .

2. Invert the two equations by introducing the inverse resistivity tensors $\hat{\rho}_1^{-1}$ and $\hat{\rho}_2^{-1}$; write the equation giving the total current as a function of the applied field as a function of the total resistivity tensor $\hat{\rho}^{-1}$. What is the relation between $\hat{\rho}^{-1}$ and $\hat{\rho}_1^{-1}$ and $\hat{\rho}_2^{-1}$?
3. By explicitly inverting the resistivity tensors Find the components of $\hat{\rho}^{-1}$; calculate the total magnetoresistance $\Delta\rho = \rho(H) - \rho(H = 0)$, where H is the magnetic field.
4. Calculate the total Hall coefficient for the system. If the two mobilities are equal what is the value of the Hall coefficient? Why?

5.2 Divalent impurities

(10 pts)

Consider a semiconductor with a dielectric constant $\epsilon = 12.5$ and a conduction effective mass $m = 0.067m_e$, doped with few divalent donors, that can thus be regarded as independent. Remember that the total binding energy of the He atom is $E = 5.81 Ry$.

1. Write the expression and the numerical value (in eV) of the binding energy ϵ_1 , respect to the conduction band, for a single electron on the donor.
2. Write the expression and the numerical value (in eV) of the binding energy ϵ_2 , after the addition of a second electron on the donor.
3. Estimate the effective Bohr radius (in Å) of the impurity with one electron and judge if the "hydrogenic" approximation is reasonable. Do you expect that with two electrons the approximation gets better or worse?
4. Compute the average occupation of these (independent) donor by computing a suitable average. How much is it at $T = 0$?
5. Determine the position of the chemical potential at $T \rightarrow 0$, in the hypothesis that only the mentioned donors contribute.
6. If N_d is the density of the donor dopants and one adds (monovalent) acceptor dopants as well with density $N_a = N_d$, where will the chemical potential will go as $T \rightarrow 0$?

5.3 Transport properties in gapped Graphene

(10 pts)

The bandstructure of graphene is well described by the tight-binding approximation. The peculiar degeneracy of energies at the six points in the reciprocal lattice (i.e. the vertex of the hexagonal FBZ constituting the Fermi surface) leads to a linear energy dispersion around those points, $E(\mathbf{k}) = \hbar v_F |\mathbf{k}|$.

Around k_0 , i.e. one of the six points belonging to the degeneracy the Fermi energy is at $E_F = 0$ and the Fermi velocity is about 10^6ms^{-1} . The excitations around the Fermi energy are well described by an effective 2x2 Hamiltonian:

$$\mathcal{H} = \begin{pmatrix} 0 & \hbar v_F (\hat{k}_x - i\hat{k}_y) \\ \hbar v_F (\hat{k}_x + i\hat{k}_y) & 0 \end{pmatrix}$$

Here the reduced wavenumber is $\mathbf{k} = \mathbf{k}' - \mathbf{k}_0$. Here the matrix notation describes the existence of two groups of non-equivalent Fermi points. This is called pseudospin.

1. Find the energies and wavefunctions of the electrons. Evaluate the effective mass of the excitations near Fermi energy.

[Hint: \hat{k}_x and \hat{k}_y are operators! Therefore the eigenfunctions are written as $\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}$, with ψ_+ 2D spatial wavefunctions. To treat the problem, first choose a suitable base for the spatial part in which the operator \mathcal{H} reduces to a numerical matrix. Then proceed to its diagonalization.]

2. Calculate the 2D density of states $g_0(\epsilon)$ of the excitations near Fermi energy.

Let us switch on an interaction that mixes the two pseudospin states in this way:

$$\mathcal{H}_\Delta = \begin{pmatrix} \Delta & \hbar v_F (k_x - ik_y) \\ \hbar v_F (k_x + ik_y) & -\Delta \end{pmatrix}$$

3. Find the energy eigenvalues. What happens to the band dispersion around Fermi?
4. Calculate the effective mass tensor and the density of states $g_\Delta(\epsilon)$ for the gapped system. Study the limit for $\Delta \rightarrow 0$.
5. Give an expression the diagonal components of the conductivity tensor in 2D

$$\hat{\sigma}_{ij} = -e^2 \int \frac{d\mathbf{k}}{2\pi^2} g_\Delta(\epsilon) \left(\frac{\partial f_0}{\partial \epsilon} \right) \tau(\mathbf{k}) v_i(\mathbf{k}) v_j(\mathbf{k})$$

for a gapped graphene sheet. In doing that you should bring out the density of state and the relaxation time and evaluate them at a specific energy. Which one? Why? Study the limit for $\Delta \rightarrow 0$.

6. Using the formal results from the Sommerfeld Expansion study the behavior of the conductivity for $T > 0$.