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WS14/15 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-plan electric field and current:

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

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.)

   a.   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 j_1 and j_2.

   Solution: The common electric field will be proportional to the two currents through the conductivity tensor:

$$E = \hat{\rho}_1 j_1$$
$$E = \hat{\rho}_2 j_2.$$

b. 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 $\hat{\rho}_2^{-1}$?

Solution: The total current is linked to the field through the total resisitivity tensor $\hat{\rho}$:
$$E = \hat{\rho}(j_1 + j_2)$$
By inverting the equations found in the preceding point to express j_1 and j_2 as a function of $\hat{\rho}_2^{-1}$ and $\hat{\rho}_1^{-1}$ we obtain:
$$E = \hat{\rho}\left(\hat{\rho}_1^{-1} + \hat{\rho}_2^{-1}\right)E$$
This is to say that $\hat{\rho}\left(\hat{\rho}_1^{-1} + \hat{\rho}_2^{-2}\right) = 1$, therefore we have:
$$\hat{\rho}^{-1} = \hat{\rho}_1^{-1} + \hat{\rho}_2^{-1}.$$

c. 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.

Solution: the resistivity tensor for the electron is
$$\hat{\rho}_1 = \begin{pmatrix} \rho_1 & -R_H H \\ R_H H & \rho_1 \end{pmatrix}.$$
The inverted tensor is:
$$\hat{\rho}_1^{-1} = \frac{1}{\rho_1^2 + R_H^2 H^2}\begin{pmatrix} \rho_1 & R_H H \\ -R_H H & \rho_1 \end{pmatrix}.$$
For the holes the mobility is different and the signs of the off-diagonal components is inverted (same density n but opposite charge):
$$\hat{\rho}_2^{-1} = \frac{1}{\rho_2^2 + R_H^2 H^2}\begin{pmatrix} \rho_2 & -R_H H \\ R_H H & \rho_2 \end{pmatrix}.$$
The total inverted resistivity tensor is
$$\hat{\rho}^{-1} = \begin{pmatrix} \alpha & \beta \\ -\beta & \alpha \end{pmatrix}.$$
where
$$\alpha = \frac{\rho_1}{\rho_1^2 + R_H^2 H^2} + \frac{\rho_2}{\rho_2^2 + R_H^2 H^2}$$
$$\beta = R_H H\left(\frac{1}{\rho_1^2 + R_H^2 H^2} - \frac{1}{\rho_2^2 + R_H^2 H^2}\right).$$
To find the resistivity we need to invert the tensor.
$$\hat{\rho} = \frac{1}{\alpha^2 + \beta^2}\begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix}.$$
The determinant of the matrix can be written as
$$\alpha^2 + \beta^2 = \frac{(\rho_1 + \rho_2)^2}{(\rho_1^2 + R_H^2 H^2)(\rho_2^2 + R_H^2 H^2)}$$
The total resistivity is given by the diagonal elements of the resistivity matrix:
$$\rho(H) = \frac{\alpha}{\alpha^2 + \beta^2} = \cdots = \frac{\rho_1}{(1 + \rho_1/\rho_2)^2} + \frac{\rho_2}{(1 + \rho_2/\rho_1)^2} + \frac{R_H^2 H^2}{\rho_1 + \rho_2}.$$

Therefore the magnetoresistance is given by

$$\Delta\rho(H) = \rho(H) - \rho(H = 0) = \frac{R_H^2 H^2}{\rho_1 + \rho_2}.$$

d. Calculate the total Hall coefficient for the system. If the two mobilities are equal what is the value of the Hall coefficient? Why?

Solution: The Hall coefficient is given by the non-diagonal element of the total resistivity matrix

$$R_H(H) = -\frac{\beta}{\alpha^2 + \beta^2} = \cdots = R_H H \frac{\rho_1^2 - \rho_2^2}{(\rho_1 + \rho_2)^2} = R_H H \frac{\rho_1 - \rho_2}{\rho_1 + \rho_2}.$$

If the two mobilities are equal then $\rho_1 = \rho_2$, therefore the Hall coefficient vanishes as $\rho_1 - \rho_2$.

5.2   Divalent impurities   (10 pts)

Consider a semiconductior with a dielectric constant $\epsilon = 12.5$ and a conduction effective mass $m = 0.067 m_e$, 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.

   [For a single electron the energy is the energy for the He⁺ (Z=2) atom, renormalized with the dielectric constant (from Ashcroft eq. 28.29). $\epsilon_1 = \frac{m^*}{m_e} \frac{Z^2}{\epsilon^2} \times 13.6\ \text{eV} = 0.067 \times 0.1024 \times 13.6 = 93.3\ \text{meV}.$]

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.

   [The binding energy (with respect to the conduction band bottom) we have to renormalize the He atom binding energy in the same way we did above: $\epsilon_2 = \frac{m^*}{m_e} \frac{Z^2}{\epsilon^2} \times 5.81 \times 13.6\ \text{eV} = 542\ \text{meV}.$]

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?

   [The Bohr radius is renormalized in the following way $r_0 = \frac{m_e}{m^*} \frac{\epsilon}{Z} a_0 = 14.9 \times 6.25 \times 0.53\ \text{Å} = 49.4\ \text{Å}.$ The Bohr radius The average atomic radius will increase when we add another electron, basically up to around 100 Å. The approximation is just reasonable for one electron

4. Compute the average occupation of these (independent) donor by computing a suitable average. How much is it at $T = 0$?

   [The average occupation of the Donor state is
   $$\langle n_d \rangle = \frac{2N_d}{\frac{1}{2} e^{\beta(\epsilon_2 - \mu)} + 1}$$
   Here N_d is the impurity density. At T=0 the donor density is simply twice the impurity density.]

5. Determine the position of the chemical potential at $T \to 0$, in the hypothesis that only the mentioned donors contribute

   [If only donors contribute then (Ashcroft 28.39) we have
   $$\frac{2N_d}{n_i} = 2 \sinh \beta(\mu - \mu_i) \approx \exp \beta(\mu - \mu_i)$$
   By inverting we have
   $$\mu = \mu_i + k_B T \log(2 \, N_d / n_i)$$
   Here we have assumed that the effective mass difference between the conduction and valence band is null.]

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 $T \to 0$?

   [In that case we have to substitute the donor densitites with the difference between donor and acceptor centers, each weighted by their valence. Therefore we have
   $$\mu = \mu_i + k_B T \log(N_d / n_i).$$
   ]

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 $10^6 \mathrm{ms}^{-1}$. The excitations around the Fermi energy are well described by an effective 2x2 Hamiltonian:

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

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

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

   [Hint: $\hat{k}_x$ and $\hat{k}_y$ are operators! Therefore the eigenfuctions 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.]

   [The Hamiltonian is a linear tensor function of the momentum operator $\hat{\mathbf{k}} = (\hat{k}_x, \hat{k}_y)$. Therefore we can look for the eigenvectors of the form $\begin{pmatrix} \alpha \\ \beta \end{pmatrix} e^{i\mathbf{k}\cdot\mathbf{r}}$. On this basis we reduce to a numerical C-matrix in which the operators $\hat{k}_x, \hat{k}_y$ reduce to their eigenvalues k_x, k_y:

   $$\mathcal{H} = \begin{pmatrix} 0 & \hbar v_F(k_x - ik_y) \\ \hbar v_F(k_x + ik_y) & 0 \end{pmatrix}$$

   We can find the eigenvalues by solving the secular equation

   $$\det(\mathcal{H} - E\mathbb{I}) = E^2 - \hbar^2 v_F^2 k^2 = 0$$

   Consequently we find $E = \pm\hbar v_F k$, i.e. the excitations have a linear dispersion around E=0, (The Dirac point, coincident with Fermi energy in this case.) The effective mass would appear to be infinite (since the second derivative of the energy with respect to the momentum is zero, but that definition applies only to excitations with finite mass (where we can invert the equation $\hbar k = mv^2$). Instead a linear dispersion resembles the photon momentum-energy dispersion. Therefore we can say that these excitations have zero mass.]

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

   [The density of states is $g_0(\epsilon) = \frac{1}{2\pi^2} \int d\mathbf{k}\, \delta(\epsilon \mp \hbar v_F k) = \frac{1}{\pi} \int dk\, k\, \delta(\epsilon \mp \hbar v_F k) = \frac{1}{\pi(\hbar v_F)^2} \int dt\, \text{sign}(t)\, t\, \delta(\epsilon - t) = \frac{|\epsilon|}{\pi(\hbar v_F)^2}$.
   The DOS is linear and vanishing at the Dirac point.]

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?

   [Same consideration as in point 1. The secular equation is now $E^2 - \Delta^2 - \hbar^2 v_F^2 k^2 = 0$. Therefore we have

   $$E_\Delta(\mathbf{k}) = \pm\sqrt{\Delta^2 + \hbar^2 v_F^2 k^2}.$$

   We can see that the interaction opens a Gap at Fermi (Total gap 2Δ)]

4. Calculate the effective mass tensor and the density of states $g_\Delta(\epsilon)$ for the gapped system. Study the limit for $\Delta \to 0$.

[The excitations acquire an effective mass near Fermi as

$$m_\Delta = \hbar^2 \left(\frac{\partial^2 E_\Delta}{\partial k^2} \bigg|_{k=0} \right)^{-1} = \pm \frac{|\Delta|}{v_F^2}$$

The mass tensor is diagonal and spherically symmetric. This confirms that for the ungapped graphene the mass is zero.

The density of states is $g_\Delta(\epsilon) = \frac{1}{2\pi^2} \int d\mathbf{k}\, \delta(\epsilon - E_\Delta) = \frac{1}{\pi} \int d\mathbf{k}\, k\, \delta(\epsilon - E_\Delta) =$

$$= \frac{1}{\pi(\hbar v_F)^2} \int_\Delta^\infty dt\, \text{sign}(t)\, t\, \delta(\epsilon - t) = \begin{cases} \dfrac{|\epsilon|}{\pi(\hbar v_F)^2} & |\epsilon| > \Delta \\ 0 & |\epsilon| < \Delta \end{cases}$$

I.e. the DOS functional shape is unchanged! (Apart for the gap opening)

5. Remembering Exercise 4.3, give an expression the diagonal components of the conductivity tensor in 2D 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 $\Delta \to 0$

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

[At T=0 the derivative of the dispersion is a Dirac delta. By applying the chain rule we obtain

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

$$= -\frac{e^2}{2\pi^2} \int d\mathbf{k}\, g_\Delta(\epsilon) \delta(\epsilon - \epsilon_F)\, \tau(\mathbf{k}) v_i(\mathbf{k}) v_j(\mathbf{k})$$

We can now calculate the diagonal components of the conduction tensor; the Dirac delta simply restrics the integration over the Fermi Surface:

$$\hat{\sigma}_{ii} = -\frac{e^2}{2\pi^2} g_\Delta(\epsilon_F) \tau(\epsilon_F) \int dS_F v_i^2(\mathbf{k}) = -\frac{e^2}{2\pi^2} S_F g_\Delta(\epsilon_F) \tau(\epsilon_F) \frac{v^2(\epsilon_F)}{3}.$$

Here we used the spherical symmetry of the dispersion.

$$\hat{\sigma}_{ii} = -\frac{e^2}{2\pi^2} S_F g_\Delta(\epsilon_F) \tau(\epsilon_F) \frac{v_F^2}{3} \frac{\epsilon_F^2 - \Delta^2}{\epsilon_F^2}.$$

On the Fermi surface $S_F = \pi k_F^2 = \pi \frac{\epsilon_F^2 - \Delta^2}{\hbar^2 v_F^2}$ Moreover $v^2 = \hbar^{-2} \left(\frac{\partial \epsilon}{\partial k} \right)^2 = \frac{\hbar^2 v_F^4 k^2}{\Delta^2 + \hbar^2 v_F^2 k^2} = \frac{\hbar^2 v_F^4 k^2}{\Delta^2 + \hbar^2 v_F^2 k^2}$. Then $v^2(\epsilon_F) = v_F^2 \frac{\epsilon_F^2 - \Delta^2}{\epsilon_F^2}$.

Let's examine our result a bit. For the exact system we have $\epsilon_F = 0$, and $g_\Delta(0) = 0$, For any gap value. So why bother at all? The fact is that in reality, Graphene is almost always doped, either p or n. This means that Fermi energy is either above or below the Dirac point - or the bandgap extremum in the gapped system [$\epsilon_F > \Delta$]. This gives a non-vanishing value for the DOS, the Fermi Surface area and the velocity values.

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

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

Let´s change the variable from k to the energy: $k = \frac{\sqrt{\Delta^2-\epsilon^2}}{\hbar v_F}$, and $dk = \frac{\epsilon d\epsilon}{\hbar v_F\sqrt{\Delta^2-\epsilon^2}}$. Therefore, considering the diagonal component:

$$\hat{\sigma}_{ii} = -\frac{e^2\tau}{3\pi(\hbar v_F)^2}\int_\Delta^\infty d\epsilon\,\frac{\partial f_T}{\partial \epsilon}\epsilon\, g_\Delta(\epsilon)v^2(\epsilon_F) = -\frac{e^2\tau}{\pi^2\hbar^4}\int_\Delta^\infty d\epsilon\,\frac{\partial f_T}{\partial \epsilon}(\epsilon^2-\Delta^2)$$

In general, the integral is of the form $I(\mu) = \int_0^\infty d\epsilon\frac{\partial f_T}{\partial \epsilon}\varphi(\epsilon)$. We can write this integrals in term of an integral involving the Fermi dispersion, Now by integrating by parts the integral and by considering that $\lim_{\epsilon\to\infty} f_T = 0$ and $\lim_{\epsilon\to 0}\varphi = 0$, we

$$I(\mu) = \int_0^\infty d\epsilon\,\frac{\partial f_T}{\partial \epsilon}\varphi(\epsilon) = f_T(\epsilon)\varphi(\epsilon)|_0^\infty - \int_0^\infty d\epsilon\, f_T(\epsilon)\frac{\partial \varphi}{\partial \epsilon}(\epsilon) = -\int_0^\infty d\epsilon\, f_T(\epsilon)\frac{\partial \varphi}{\partial \epsilon}.$$

This integral is now a Sommerfeld integral. Therefore we can apply the Sommerfeld expansion to the integral (Ashcroft eq. 2.70 and appendix C)

$$I(\mu) = \varphi(\mu) + \frac{\pi^2}{6}(k_B T)^2\varphi''(\mu) + O\left(\frac{k_B T}{\mu}\right)^4.$$

We can then expand the functions around ϵ_F in order to take into account the variations of the chemical potential:

$$I(\mu) = \varphi(\epsilon_F) + (\mu-\epsilon_F)\varphi'(\epsilon_F) + \frac{\pi^2}{6}(k_B T)^2[\varphi''(\epsilon_F) + (\mu-\epsilon_F)\varphi'''(\epsilon_F)] + O\left(\frac{k_B T}{\mu}\right)^4.$$

Now in order to correctly evaluate the integral we have to also evaluate the variation of the chemical potential with the temperature (Ashcroft eq. 2.77)

$$\mu = \epsilon_F - \frac{\pi^2}{6}(k_B T)^2\frac{g_\Delta'(\epsilon_F)}{g_\Delta(\epsilon_F)} + O\left(\frac{k_B T}{\mu}\right)^4$$

By substituting this above and getting the power two on we finally get:

$$I(\mu) = \varphi(\epsilon_F) - \frac{\pi^2}{6}(k_B T)^2\left[\frac{g_\Delta'(\epsilon_F)}{g_\Delta(\epsilon_F)}\varphi'(\epsilon_F) + \varphi''(\epsilon_F)\right] + O\left(\frac{k_B T}{\mu}\right)^4.$$

And by evaluating the derivative we get:

$$\hat{\sigma}_{ii}(T) = \hat{\sigma}_{ii} - \frac{\pi^2}{3}\frac{e^2\tau}{\pi^2\hbar^4}(k_B T)^2 + O\left(\frac{k_B T}{\mu}\right)^4.$$

If $\epsilon_F < \Delta$, and

$$\hat{\sigma}_{ii}(T) = \hat{\sigma}_{ii} - \frac{2\pi^2}{3}\frac{e^2\tau}{\pi^2\hbar^4}(k_B T)^2 + O\left(\frac{k_B T}{\mu}\right)^4.$$

If $\epsilon_F > \Delta$.