

Solid state physics (TN2844) 2025

Final exam (180 minutes)

May 20, 2025

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- If these solutions contain mistakes (and they may), the physical correctness has priority over them in grading.
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This exam is designed and reviewed by A. Akhmerov and T. van der Sar

1. 1D continuum model with spin-orbit coupling and magnetic field

We consider a 1D Hamiltonian:

$$H(k) = \begin{pmatrix} \frac{\hbar^2}{2m}(k+k_0)^2 & B \\ B & \frac{\hbar^2}{2m}(k-k_0)^2 \end{pmatrix} \equiv \frac{\hbar^2}{2m}(k^2+k_0^2) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} \hbar^2 k_0 k / m & B \\ B & -\hbar^2 k_0 k / m \end{pmatrix},$$

where the two states are the spin-up and spin-down states of electrons in the system. Here $k_0 > 0$ is a momentum shift, B is the spin coupling due to the magnetic field, k is the 1D wave vector, and m is the effective mass. Two equivalent ways of writing this Hamiltonian are presented above for your convenience.

- (a) (5 points) Compute the dispersion relation of this system.

Solution: For the general case with finite B , we need to diagonalize the Hamiltonian:

$$H(k) = \begin{pmatrix} \frac{\hbar^2}{2m}(k+k_0)^2 & B \\ B & \frac{\hbar^2}{2m}(k-k_0)^2 \end{pmatrix}$$

For convenience, let's define $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$ and $\Delta_k = \frac{\hbar^2 k_0 k}{m}$. Then the Hamiltonian can be written as:

$$H(k) = \begin{pmatrix} \varepsilon_k + \Delta_k + \frac{\hbar^2 k_0^2}{2m} & B \\ B & \varepsilon_k - \Delta_k + \frac{\hbar^2 k_0^2}{2m} \end{pmatrix}$$

The eigenvalues are:

$$E_{\pm}(k) = \varepsilon_k + \frac{\hbar^2 k_0^2}{2m} \pm \sqrt{\Delta_k^2 + B^2} = \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2 k_0^2}{2m} \pm \sqrt{\left(\frac{\hbar^2 k_0 k}{m}\right)^2 + B^2}$$

At $B = 0$, these simplify to:

$$E_{\pm}(k) = \frac{\hbar^2}{2m}(k \pm k_0)^2$$

- (b) (10 points) Compute the effective mass m^* at finite B for both bands at $k = 0$. Hint: first expand the dispersion relation around $k = 0$.

Solution: Following the hint, let's start by using the dispersion relation from part (a) and expand it around $k = 0$:

$$E_{\pm}(k) = \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2 k_0^2}{2m} \pm \sqrt{\left(\frac{\hbar^2 k_0 k}{m}\right)^2 + B^2}$$

For small k values, we can expand the square root term using the Taylor series approximation:

$$\sqrt{a^2 + b^2} \approx b + \frac{a^2}{2b} + \dots$$

Applying this to our dispersion relation:

$$E_{\pm}(k) \approx \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2 k_0^2}{2m} \pm \left[B + \frac{1}{2B} \left(\frac{\hbar^2 k_0 k}{m} \right)^2 \right] = E_{\pm}(0) + \frac{\hbar^2 k^2}{2m} \left(1 \pm \frac{\hbar^2 k_0^2}{Bm} \right)$$

The effective mass is defined as:

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{d^2 E}{dk^2}$$

From our expansion, we can directly read off:

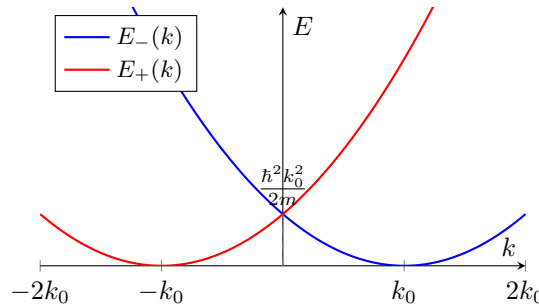
$$\frac{1}{m_{\pm}^*} = \frac{1}{\hbar^2} \cdot \frac{\hbar^2}{m} \left(1 \pm \frac{\hbar^2 k_0^2}{Bm} \right) = \frac{1}{m} \left(1 \pm \frac{\hbar^2 k_0^2}{Bm} \right)$$

(c) (15 points) Consider $B = 0$, when the Hamiltonian is diagonal. Hint: your answer from part (a) is not convenient for this question.

- Sketch the dispersion relation.
- Based on your sketch, sketch the density of states $g(E)$.
- Compute the expression for $g(E)$. Hint: consider if the density of states depends on k_0 .
- Sketch the density of states for the lower band $g_-(E)$.

Solution:

Sketch of the dispersion relation:



Based on the sketch, sketch the density of states $g(E)$:

Compute the expression for $g(E)$:

At $B = 0$ the Hamiltonian is diagonal, so the two spin branches are two identical parabolas shifted in opposite directions in momentum. A momentum shift does not change the density of states, so the total density of states per unit length is exactly the same as that of the 1D free electron model with two spin branches:

$$g(E) = \frac{2}{\pi \hbar} \sqrt{\frac{m}{2E}}$$

where the factor of 2 accounts for the two shifted branches.

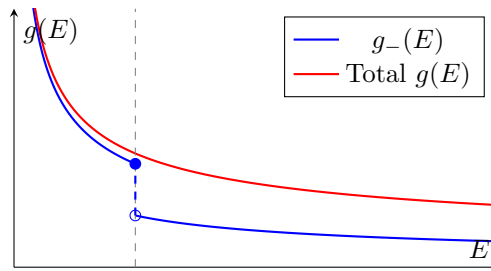
The total density of states is due to 4 equal contributions: two branches and two signs of the group velocity.

For the lower eigenvalue $E_-(k)$, the two shifted parabolas cross at $k = 0$ and $E_0 = \frac{\hbar^2 k_0^2}{2m}$. Below E_0 , all 4 solutions at a given energy belong to the lower eigenvalue. Above E_0 , only 2 of them do; the other 2 belong to the upper eigenvalue.

Sketch the density of states for the lower band $g_-(E)$:

Therefore the density of states for the lower band is:

$$g_-(E) = \begin{cases} \frac{2}{\pi\hbar} \sqrt{\frac{m}{2E}} & E < \frac{\hbar^2 k_0^2}{2m} \\ \frac{1}{\pi\hbar} \sqrt{\frac{m}{2E}} & E > \frac{\hbar^2 k_0^2}{2m} \end{cases}$$



The lower band DOS shows a characteristic $1/\sqrt{E}$ behavior with a step discontinuity at $E_0 = \frac{\hbar^2 k_0^2}{2m}$, dropping by a factor of 2 when the upper band becomes accessible.

- (d) (10 points) Determine how the electron heat capacity scales with temperature and with Fermi energy at $B = 0$ when $T \rightarrow 0$.

Solution: For a fermionic system in the low temperature limit, the electronic heat capacity can be estimated based on the free electron model.

$$C_V \propto k_B^2 T \cdot g(E_F)$$

Substituting our expression for the density of states:

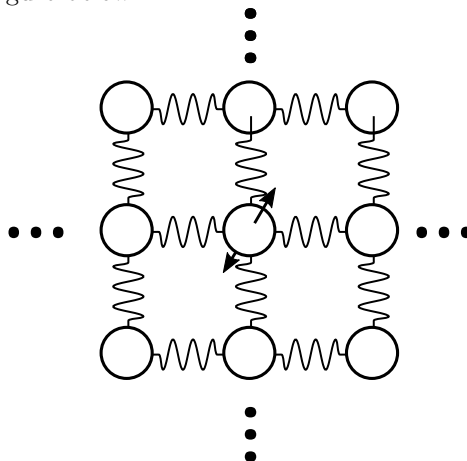
$$C_V \propto k_B^2 T \cdot \frac{2m}{\pi\hbar^3 \sqrt{2mE_F}}$$

This gives us the scaling relations:

- $C_V \propto T$
- $C_V \propto \frac{1}{\sqrt{E_F}}$

2. Vibrations of a membrane

We consider a square lattice of atoms that are connected by springs and move in the direction z perpendicular to the plane, as shown in the figure below.



The lattice constant is a , the mass of each atom is m , and the returning force acting on the atom with

displacement u_1 and connected to another atom with displacement u_2 is equal to $\kappa(u_1 - u_2)$.

- (a) (10 points) Write down the equations of motion of the atom in the unit cell with indices n, m (i. e. with displacement $u_{n,m}$).

Solution:

$$m\ddot{u}_{n,m} = \kappa(u_{n+1,m} + u_{n-1,m} + u_{n,m+1} + u_{n,m-1} - 4u_{n,m})$$

- (b) (10 points) Write down the appropriate plane wave ansatz, substitute it into the equations of motion, and compute the dispersion relation. Check that if $k_y = 0$ (where k_y is the y -component of the wave vector) you reproduce the dispersion relation of an atomic chain.

Solution:

$$u_{n,m} = Ae^{i(k_x na + k_y ma + \omega t)}$$

$$m\omega^2 = \kappa(4 - e^{ik_x a} - e^{-ik_x a} - e^{ik_y a} - e^{-ik_y a})$$

$$\omega = 2\sqrt{\frac{\kappa}{m}} \sqrt{\sin^2(k_x a/2) + \sin^2(k_y a/2)}$$

- (c) (10 points)

- What is the sound velocity in this membrane?
- Compute the density of states at $\omega \ll \sqrt{\kappa/m}$.

Solution:

$$v_s = a\sqrt{\kappa/m}.$$

There is only one polarization, and therefore the density of states is:

$$g(\omega) = \frac{L^2\omega}{2\pi v_s^2}.$$

- (d) (10 points)

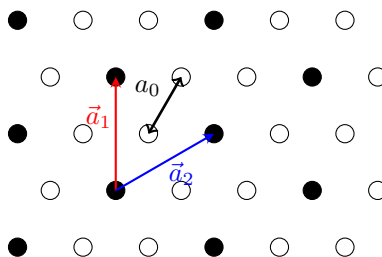
- If the lattice constant in x -direction was changed to $2a$, argue what would happen to the sound velocity in x - and y -direction?
- If the spring constant κ in x -direction was doubled, argue what would happen to the sound velocity in x - and y -direction?

Solution: If the lattice constant in x -direction would be doubled, so would the sound velocity in x -direction, while the velocity in y -direction would stay untouched.

If the spring constant κ in x -direction was doubled, the sound velocity in x -direction would increase by a factor of $\sqrt{2}$, while the velocity in y -direction would stay untouched.

3. Crystal structure

Consider the following 2D crystal structure with two types of atoms and the distance a_0 between all neighboring atoms.



- (a) (10 points) Draw primitive lattice vectors on the crystal structure above. Then determine the distance between the lattice points and express the primitive lattice vectors in Cartesian coordinates. Finally, write down the basis of the unit cell.

Solution:

$$\vec{a}_1 = (0, a) = (0, \sqrt{3}a_0)$$

$$\vec{a}_2 = \left(\frac{\sqrt{3}a}{2}, \frac{a}{2} \right) = \left(\frac{3a_0}{2}, \frac{\sqrt{3}a_0}{2} \right)$$

$$|\vec{a}_1| = |\vec{a}_2| = a = \sqrt{3}a_0$$

$$\vec{r}_0 = (0, 0) \quad (\text{black atom at lattice point})$$

$$\vec{r}_1 = \left(\frac{1}{3}, \frac{1}{3} \right) \quad (\text{white atom})$$

$$\vec{r}_2 = \left(\frac{2}{3}, \frac{2}{3} \right) \quad (\text{white atom})$$

- (b) (10 points)

- Compute the reciprocal lattice vectors of this crystal structure.
- Calculate the structure factor for this lattice, assuming that the black atoms have structure factor f_A and the white atoms have structure factor f_B .

Solution: Reciprocal lattice vectors: The lattice is the same as that of the honeycomb lattice in the lecture notes.

$$\vec{b}_1 = \frac{4\pi}{3a_0} \begin{pmatrix} \frac{1}{\sqrt{3}} \\ -1 \end{pmatrix}$$

$$\vec{b}_2 = \frac{4\pi}{3a_0} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Structure factor:

$$S(h, k) = f_A + f_B \left[e^{2\pi i \frac{h+k}{3}} + e^{2\pi i \frac{2(h+k)}{3}} \right]$$

- (c) (10 points) Determine if any diffraction peaks are absent when $f_A \neq f_B$ and when $f_A = f_B$.

Solution:

For general f_A and f_B , no peaks are absent.

When $f_A = f_B$: Peaks are absent when $(h + k)$ is not divisible by 3

4. Two-valence band 2D semiconductor

Consider a strictly **two-dimensional** semiconductor with a conduction band and two valence bands. The Hamiltonian near the band extrema can be written as $H_c(\vec{k}) = E_C + \frac{\hbar^2 k^2}{2m_c}$ for the conduction band, and $H_{v1}(\vec{k}) = E_{V,1} - \frac{\hbar^2 k^2}{2m_1}$, $H_{v2}(\vec{k}) = E_{V,2} - \frac{\hbar^2 k^2}{2m_2}$ for the two valence bands. The energy separation between the valence bands is $\Delta = E_{V,1} - E_{V,2} > 0$, and the energy gap $E_G = E_C - E_{V,1} \gg k_B T$. The effective masses satisfy $m_1 > m_2$.

- (a) (10 points) Calculate and sketch the density of states $g(E)$ of this semiconductor. Clearly indicate the contribution from each band and the relevant energy scales on your sketch.

Solution: For a 2D system, the density of states for each band is constant within its energy range:

For the conduction band:

$$g_c(E) = \frac{m_c}{\pi\hbar^2} \cdot \Theta(E - E_C)$$

For the first valence band:

$$g_{v1}(E) = \frac{m_1}{\pi\hbar^2} \cdot \Theta(E_{V,1} - E)$$

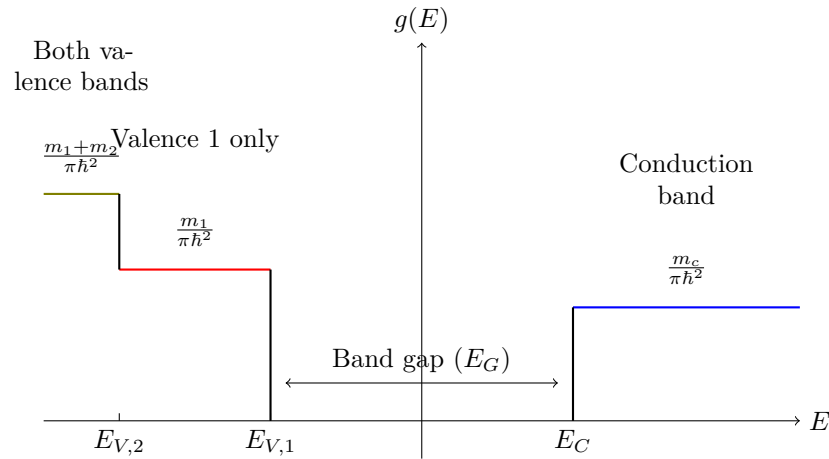
For the second valence band:

$$g_{v2}(E) = \frac{m_2}{\pi\hbar^2} \cdot \Theta(E_{V,2} - E)$$

where Θ is the Heaviside step function.

The total density of states is:

$$g(E) = g_c(E) + g_{v1}(E) + g_{v2}(E)$$



- (b) (10 points) Calculate the concentration of electrons in the conduction band and holes in each of the valence bands as a function of the Fermi energy E_F , temperature T , and the respective effective masses. Assume the Fermi level is in the band gap far from all bands and the Boltzmann approximation is valid.

Solution: The concentration of electrons in the conduction band is:

$$\begin{aligned} n_c &= \int_{E_C}^{\infty} g_c(E) f(E) dE \\ &\approx \frac{m_c}{\pi\hbar^2} \int_{E_C}^{\infty} e^{-(E-E_F)/k_B T} dE \\ &= \frac{m_c}{\pi\hbar^2} \cdot k_B T \cdot e^{-(E_C-E_F)/k_B T} \end{aligned}$$

The concentration of holes in the first valence band is:

$$\begin{aligned} n_{v1} &= \int_{-\infty}^{E_{V,1}} g_{v1}(E) [1 - f(E)] dE \\ &\approx \frac{m_1}{\pi\hbar^2} \int_{-\infty}^{E_{V,1}} e^{(E-E_F)/k_B T} dE \\ &= \frac{m_1}{\pi\hbar^2} \cdot k_B T \cdot e^{(E_{V,1}-E_F)/k_B T} \end{aligned}$$

Similarly, the concentration of holes in the second valence band is:

$$\begin{aligned} n_{v2} &= \frac{m_2}{\pi\hbar^2} \cdot k_B T \cdot e^{(E_{V,2}-E_F)/k_B T} \\ &= \frac{m_2}{\pi\hbar^2} \cdot k_B T \cdot e^{(E_{V,1}-E_F-\Delta)/k_B T} \\ &= \frac{m_2}{\pi\hbar^2} \cdot k_B T \cdot e^{(E_{V,1}-E_F)/k_B T} \cdot e^{-\Delta/k_B T}. \end{aligned}$$

- (c) (10 points) First, derive the charge neutrality condition for this semiconductor. Then, solve for the equilibrium Fermi energy E_F in the intrinsic case when $\Delta \gg k_B T$. Finally, determine the concentrations of electrons and holes in each band.

Solution: The charge neutrality condition for this semiconductor is:

$$n_c = n_{v1} + n_{v2}$$

Substituting the expressions we derived:

$$\frac{m_c}{\pi\hbar^2} \cdot k_B T \cdot e^{-(E_C-E_F)/k_B T} = \frac{m_1}{\pi\hbar^2} \cdot k_B T \cdot e^{(E_{V,1}-E_F)/k_B T} + \frac{m_2}{\pi\hbar^2} \cdot k_B T \cdot e^{(E_{V,1}-E_F-\Delta)/k_B T}$$

Simplifying and using $E_G = E_C - E_{V,1}$:

$$m_c \cdot e^{-(E_C-E_F)/k_B T} = \left(m_1 + m_2 e^{-\Delta/k_B T}\right) e^{(E_{V,1}-E_F)/k_B T}.$$

This can be rewritten as:

$$e^{2E_F/k_B T} = \frac{m_1 + m_2 e^{-\Delta/k_B T}}{m_c} e^{(E_C+E_{V,1})/k_B T}.$$

Since $\Delta \gg k_B T$, the contribution from the second valence band is smaller by a factor of $e^{-\Delta/k_B T} \ll 1$. Therefore, we can approximate:

$$e^{2E_F/k_B T} \approx \frac{m_1}{m_c} e^{(E_C+E_{V,1})/k_B T}.$$

Solving for E_F :

$$E_F \approx \frac{E_C + E_{V,1}}{2} + \frac{k_B T}{2} \ln \left(\frac{m_1}{m_c} \right).$$

If we set $E_{V,1}$ as our reference energy (i.e., $E_{V,1} = 0$), this simplifies to:

$$E_F \approx \frac{E_G}{2} + \frac{k_B T}{2} \ln \left(\frac{m_1}{m_c} \right)$$

Now we can determine the concentrations of all particles:

The electron concentration in the conduction band is:

$$n_c \approx \frac{m_c}{\pi\hbar^2} \cdot k_B T \cdot e^{-(E_G-E_F)/k_B T} = \sqrt{\frac{m_c m_1}{(\pi\hbar^2)^2}} \cdot k_B T \cdot e^{-E_G/2k_B T}$$

The hole concentration in the first valence band is:

$$n_{v1} \approx \frac{m_1}{\pi\hbar^2} \cdot k_B T \cdot e^{(E_{V,1}-E_F)/k_B T} = \sqrt{\frac{m_c m_1}{(\pi\hbar^2)^2}} \cdot k_B T \cdot e^{-E_G/2k_B T}$$

The hole concentration in the second valence band is:

$$n_{v2} \approx \frac{m_2}{\pi\hbar^2} \cdot k_B T \cdot e^{(E_{V,2}-E_F)/k_B T} = \frac{m_2}{m_1} \cdot n_{v1} \cdot e^{-\Delta/k_B T}.$$

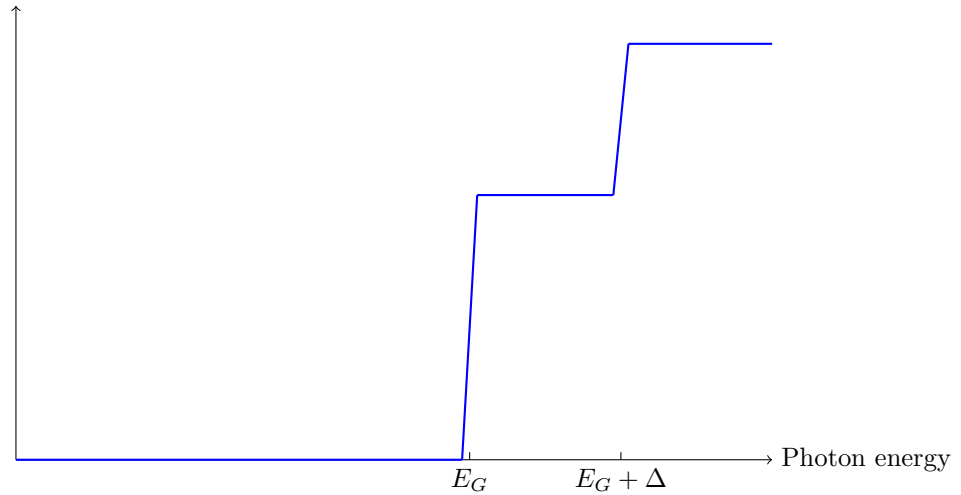
Since $\Delta \gg k_B T$, we have $n_{v2} \ll n_{v1}$, confirming our earlier approximation. The intrinsic carrier concentration is:

$$n_i \approx n_c \approx n_{v1} \approx \sqrt{\frac{m_c m_1}{(\pi\hbar^2)^2}} \cdot k_B T \cdot e^{-E_G/2k_B T}$$

(d) (10 points) Sketch the optical absorption spectrum of this semiconductor. In your sketch indicate the relevant energy scales.

Solution:

Absorption coefficient, $\alpha(\hbar\omega)$



Key features of the spectrum:

1. No absorption below E_G
2. Step increase at $\hbar\omega = E_G$ (valence band 1 to conduction band)
3. Second step increase at $\hbar\omega = E_G + \Delta$ (valence band 2 to conduction band)