

T5. Hall Effect in InSb

In a long bar having the shape of rectangular parallelepiped with sides a , b , and c ($a \gg b \gg c$), made from the semiconductor InSb flows a current I parallel to the edge a . The bar is in external magnetic field B which is parallel to the edge c . The magnetic field produced by the current I can be neglected. The current carriers are electrons. The average velocity of electrons in a semiconductor in the presence of an electric field only is $v = \mu E$, where μ is called mobility. If the magnetic field is also present, the electric field is no longer parallel to the current. This phenomenon is known as the Hall effect.

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| A1 | Determine what the magnitude and the direction of the electric field in the bar is, to yield the current described above. |
| A2 | Calculate the difference of the electric potential between the opposite points on the surface of the bar in the direction of the edge b . |
| A3 | Find the analytical expression for the DC component of the electric potential difference if the current and the magnetic field are alternating (AC); $I = I_0 \sin \omega t$ and $B = B_0 \sin(\omega t + \delta)$ |
| A4 | Design and explain the electric circuit which would make possible, by exploiting the result A3, to measure the power consumption of an electric apparatus connected with the AC network. |

The electron mobility in InSb is $7.8 \text{ m}^2\text{T/Vs}$, the electron concentration in InSb is $2.5 \cdot 10^{22} \text{ m}^{-3}$, $I = 1.0 \text{ A}$, $B = 0.10 \text{ T}$, $b = 1.0 \text{ cm}$, $c = 1.0 \text{ mm}$, $e_0 = 1.6 \cdot 10^{-19} \text{ C}$

T6. Semiconductor band gap

In this problem we will consider the structure of semiconductors from the point of view of solid-state physics and explain the temperature dependences of the concentration of electrons and holes. To describe the electrons on the upper shells of the atoms in a crystal lattice, we consider the problem of electron motion in the effective periodic potential $U(\vec{r})$, which models the interaction of the electron with the nuclei and the surrounding low-energy electrons in the nodes of the crystal lattice.

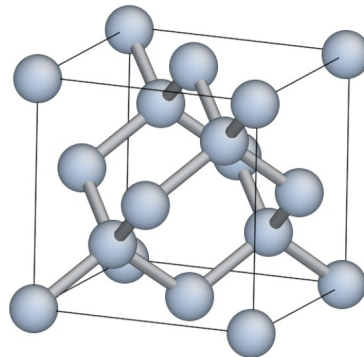
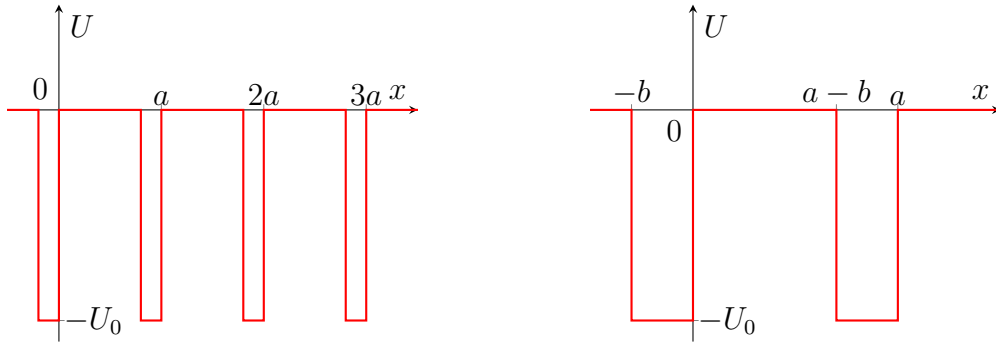


Figure 1. The crystal lattice of silicon. Wen, Mingjian et. al (2021).

Let us simplify the problem to the Kronig-Penney model (1931). Let us consider a one-dimensional problem: let non-interacting electrons move in the electric field of a chain of stationary charges located at a distance a from each other. Let $U(x)$ be the periodic potential, modeling the interaction of the electron with the crystal lattice, consist of rectangular wells of depth U_0 and width b .



From the point of view of quantum mechanics, to describe the behavior of electrons, we need to find the wave functions $\Psi(x)$ and their corresponding energies E satisfying the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\Psi''(x) + U(x)\Psi(x) = E\Psi(x).$$

Quantum mechanics requires that the derivative $\Psi'(x)$ of the wave function has no discontinuities.

Bloch's theorem allows us to significantly narrow down the set of functions among which we will search for solutions. According to this theorem, the solutions to the equation in the periodic potential $U(x)$ can only be a function of the following form:

$$\Psi(x) = e^{ikx/a}u(x/a),$$

where $k \in [-\pi, \pi]$ is a dimensionless constant called quasimomentum, and $u(y)$ is a periodic function with unit period, i.e., $u(y+1) = u(y)$.

A1 Substitute $\Psi(x) = e^{ikx/a}u(x/a)$ into the Schrödinger equation and get the equation

$$u'' + 2iku' + \left[\frac{2ma^2}{\hbar^2} (E - U(x)) - k^2 \right] u = 0$$

on $u(y)$.

Let's nondimensionalize the problem, so we introduce $2mabU_0/\hbar^2 = k_0^2$ and $Ea/(U_0b) = \varepsilon$. The values of k_0 and b/a include all physical properties of the system.

Then we have a linear differential equation with constant coefficients on $u(y)$ in each of the domains $y \in [-b/a, 0]$ and $x \in [0, 1 - b/a]$:

$$\begin{aligned} u'' + 2iku' + \left[k_0^2 \left(\varepsilon + \frac{a}{b} \right) - k^2 \right] u &= 0 \quad \text{for } y \in [-b/a, 0] \\ u'' + 2iku' + [k_0^2 \varepsilon - k^2] u &= 0 \quad \text{for } y \in [0, 1 - b/a] \end{aligned}$$

A2 Consider a linear differential equation with constant coefficients α and β :

$$u'' + 2i\alpha u' + (\beta - \alpha^2)u = 0.$$

Find the values of $\lambda_{1,2}$ for which the function $u_{1,2}(y) = e^{\lambda_{1,2}y}$ is a solution to this equation. Check that for any constants A and B , the function $u(y) = Ae^{\lambda_1 y} + Be^{\lambda_2 y}$ is also a solution to this equation.

Now we understand how the function $u(y)$ can be arranged and its form is completely given by two pairs of constants A and B (a pair on each segment):

$$\begin{aligned} u(y) = u_I(y) &= A_1 e^{\lambda_{11}y} + B_1 e^{\lambda_{12}y} \quad \text{for } y \in [-b/a, 0] \\ u(y) = u_{II}(y) &= A_2 e^{\lambda_{21}y} + B_2 e^{\lambda_{22}y} \quad \text{for } y \in [0, 1 - b/a]. \end{aligned}$$

So that $u(y)$ can be substituted into expressions for the wave function $\Psi(x) = e^{ikx/a}u(x/a)$, it remains to be required that

1. Periodicity of $u(x)$.
2. Continuity of $u(x)$ at the point $y = 0$ of the gluing solutions u_I and u_{II} .
3. Continuity of $u'(x)$ at the point $y = 0$ of the gluing solutions of u_I and u_{II} .
4. Continuity of $\Psi'(x)$ at the points $x = -b + a \cdot n$.

A3 Write a system of equations for the coefficients A_1, A_2, B_1 and B_2 corresponding to the requirements on the functions $u_I(x)$ and $u_{II}(x)$, in matrix form

$$M \begin{pmatrix} A_1 \\ A_2 \\ B_1 \\ B_2 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} & M_{13} & M_{14} \\ M_{21} & M_{22} & M_{23} & M_{24} \\ M_{31} & M_{32} & M_{33} & M_{34} \\ M_{41} & M_{42} & M_{43} & M_{44} \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ B_1 \\ B_2 \end{pmatrix} = 0.$$

Write the coefficients of the matrix M_{ij} by $\lambda_{11}, \lambda_{12}, \lambda_{21}, \lambda_{22}, a$, and b .

The system of equations for the constants $A_{1,2}, B_{1,2}$ considered above has a non-trivial solution (a solution other than $A_1 = A_2 = B_1 = B_2 = 0$) only if $\det M = 0$.

Moreover, if we require the equality $\det M = 0$ to be satisfied, we are restricted in choosing the values of $\lambda_{11}, \lambda_{12}, \lambda_{21}, \lambda_{22}$ when a and b are fixed. Recall that λ_{ij} are expressed through the physical parameter of the system k_0 and the chosen values of quasimomentum k and energy E . That is, the equation $\det M = 0$ restricts the choice of k and E . In other words, for a particular quasimomentum k the energy E cannot be any, but only some from a restricted set.

Thus, we can search for all pairs of values of energy E and quasimomentum k that we are interested in, to us and check for which of them the equation $\det M = 0$ is satisfied. This problem is computationally challenging but conceptually trivial, so we will solve it using a computer. We will consider a particular pair (k, E) as a solution of the quantum mechanical problem if the equality $\det M = 0$ is satisfied for some ε_0 : $|\det M| < \varepsilon_0$.

Exactly this algorithm is implemented in the program `energy.py`. The results are presented graphically as a plot $\varepsilon = Ea/(U_0b)$ of k , which is also called the energy spectrum. The meaning of this graph is as follows: for each value of the quasimomentum k the values of the energy E are given, which are solutions of to the Schrödinger equation, The graph is derived only for $k \in [0, \pi]$, since it is symmetric with respect to $k = 0$ and $k = \pi$.

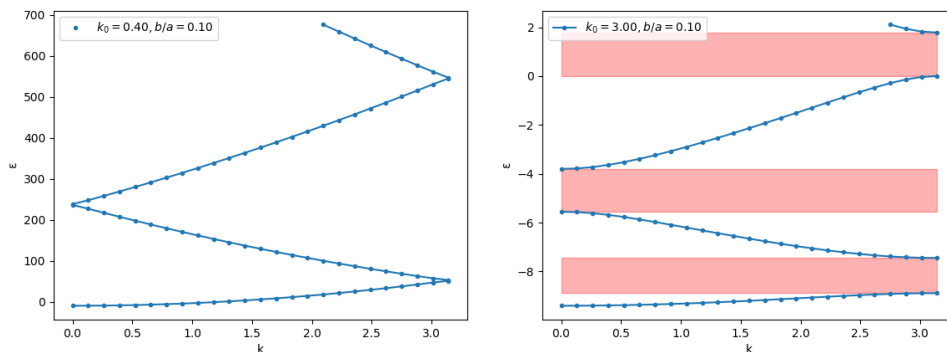


Figure 2. An example of the spectrum of ε vs. k with small (indistinguishable in the chosen scale) band gaps on the left and with large band gaps on the right (highlighted in red).

For different model parameters k_0 and b/a the energy spectrum (E, k) changes. On the left graph we see that for any energy $E > -U_0 a/b$ there is a corresponding state, i.e. the value of the quasimomentum k . On the right graph, however, we see that there are segments of energy E to which no stationary quantum states correspond, i.e. there are forbidden regions of energy E which are called band gaps.

To demonstrate the importance of band gaps for semiconductors, let us consider how the electrons are distributed among the states we have found. Recall that no two electrons can be in the same state because of the Pauli exclusion principle.

First, instead of a crystal, we consider a "box" of length L such that no electron can be outside the box (i.e., the wave function $\Psi(x)$ converges to 0 at the boundaries of the box). Inside the box, we have the Schrödinger equation

$$-\frac{\hbar^2}{2m}\Psi'' = E\Psi,$$

whose solutions are de Broglie waves $\Psi(x) = e^{ikx/a}$.

A5 Show that the de Broglie wave $\Psi(x) = e^{ikx/a}$ has the energy $E = \frac{\hbar^2 k^2}{2ma^2}$.

At the box boundaries, the wave functions must go to 0, i.e., we fit de Broglie wave functions of the following form:

$$\Psi(x) = \frac{e^{ikx/a} - e^{-ikx/a}}{2i} = \sin \frac{kx}{a}, \quad \text{where} \quad \sin \frac{kL}{a} = 0$$

so $k = \pi na/L$ where n is a natural number. If there are N electrons in the box at zero temperature (i.e., we find their collective lowest energy state), then they occupy the first N lowest energy states. Accordingly, the Fermi energy E_F is the energy of the highest level occupied by the set of electrons at zero temperature. Since that electrons have spin, two different states with opposite spin direction and the same values of k and E correspond to one pair (k, E) .

A6 Express E_F in terms of L , N , m , and $\hbar$.

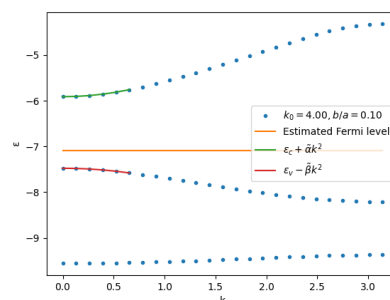
For a similar consideration of the collective behavior of electrons in the considered crystal lattice, let us place the lattice in a box, i.e., we will also require that the wave function to be zero at the boundaries of the box. The wave functions obtained by means of Bloch's theorem $e^{ikx/a}u(x/a)$ allow us to easily satisfy this requirement (if we choose constants so that $u^*(0) = u(0)$ and $u^*(L) = u(L)$, where $*$ is the complex conjugation operation):

$$\Psi(x) = u(x/a)e^{ikx/a} + u^*(x/a)e^{-ikx/a} \Rightarrow \Psi(0) = 0, \Psi(L) = 2iu(L/a)\sin(kx/a)$$

when $k = a\pi n/L$, where n is natural.

In the case of silicon, a one-dimensional crystal of length L contains L/a atoms, with each atom corresponding to 4 electrons from the outer orbitals, i.e., eventually $4L/a$ electrons are in the upper levels and so the estimate for the position of the Fermi level is:

$$E_F = \frac{2\pi^2 \hbar^2}{ma^2}, \quad \varepsilon_F = \frac{4\pi^2}{k_0^2}.$$



A7	Use the program energy.py to obtain the dependence of the band gap E_g , where the Fermi level is located, on the parameter k_0 at $b/a = 0.1$. Consider $a = 0.5$ nm, electron mass $m = 9.1 \cdot 10^{-31}$ kg, Planck constant $\hbar = 1.05 \cdot 10^{-34}$ J · s, elementary charge $e = 1.60 \cdot 10^{-19}$ C. Fill in the table.txt table and use the program bandgap.py to draw a graph of this relationship. In table.txt table, the separator between columns is tab.
A8	What k_0 corresponds to the forbidden zone of silicon $E_{\text{Si}} = 1.12$ eV? Do all further calculations for this k_0 .

If the temperature of the electrons is different from zero, the energy boundary is slightly "blurred" and a some of the electrons with energy $E < E_F$ appear in states with energy $E > E_F$. Formally, this is described as follows: if there are g different states with the same energy E , then

$$F(g, E) = \frac{g}{e^{\frac{E-E_F}{k_B T}} + 1}$$

of which on average will be filled with electrons, where $k_B = 1.38 \cdot 10^{23}$ J/K is the Boltzmann constant. As you can see at $T \rightarrow 0$ all states with $E < E_F$ are completely filled and all states with $E > E_F$ are free.

The state of electrons in a semiconductor at finite temperature is usually described in this form:

1. We first consider the electron gas at zero temperature: it completely occupies all levels with $E < E_F$.
2. The heating of the electron gas is equivalent to the appearance of excitations: electrons that have moved from the lower band (valence band) to the upper band (conduction band).
3. Such an electron transition is equivalent to adding one electron to the conduction band and adding a hole (i.e., "no" electrons) to the valence band.

We will use this approach. To do this, we need to find an approximation for the conduction band edge $E(k) = E_c + \alpha k^2$ and the valence band edge $E(k) = E_v - \beta k^2$. You can find the values $\varepsilon_c, \varepsilon_v, \tilde{\alpha} = \alpha a / (U_0 b)$, $\tilde{\beta} = \beta a / (U_0 b)$ in the output of energy.py.

A9	Use the program energy.py to find the values of $E_c - E_F$, $E_F - E_v$, α , and β . Check for yourself that $E_c - E_v = E_{\text{Si}}$. Also find the values of $(E_c - E_F)/k_B T$ and $(E_F - E_v)/k_B T$ for $T = 300$ K.
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Use the program energy.py to find the values of $E_c - E_F$, $E_F - E_v$, α , and β . Check for yourself that $E_c - E_v = E_{\text{Si}}$. Also find the values of $(E_c - E_F)/k_B T$ and $(E_F - E_v)/k_B T$ for $T = 300$ K. Earlier we obtained that, because of the "box" in which we placed the crystal, the states with any value of the quasimomentum k in the interval $[-\pi, \pi]$ are admissible, but only a discrete set of quasimomentums $k \in [0, \pi]$ differ from each other by $\Delta k = \pi a / L$. In result $g = \frac{2}{\Delta k} \left| \frac{dE}{dk} \right|^{-1} \Delta E$ of different states (with different values of quasi-momentum and spin) correspond to the domain $[E, E + \Delta E]$.

Substituting the approximation for the $E(k)$ edges of the valence band and conduction bands we get

$$g_c(\Delta E, k) = \frac{L \Delta E}{\pi a \alpha k}, \quad g_v(\Delta E, k) = \frac{L \Delta E}{\pi a \beta k}$$

Thus the total number of states filled in the conduction band:

$$\begin{aligned} n &= \sum_{E \geq E_c} F(g(\Delta E, k), E) = \sum_{E \geq E_c} \frac{g_c(\Delta E, k)}{e^{\frac{E-E_F}{k_B T}} + 1} \simeq \sum_{E \geq E_c} g_c e^{\frac{E_F-E}{k_B T}} \simeq \\ &\simeq \int_{E_c}^{+\infty} \frac{L}{\pi a \alpha k} e^{\frac{E_F-E}{k_B T}} dE = \frac{2L}{\pi a} e^{\frac{E_F-E_c}{k_B T}} \int_0^{\infty} e^{-\frac{\alpha k^2}{k_B T}} dk = \frac{L}{a} e^{\frac{E_F-E_c}{k_B T}} \sqrt{\frac{k_B T}{\pi \alpha}}. \end{aligned}$$

This number n is the number of electrons involved in the transfer processes.

A10 Show that the total number p of NOT-filled states in the valence band is

$$p = \frac{L}{a} e^{\frac{E_v - E_F}{k_B T}} \sqrt{\frac{k_B T}{\pi \beta}}.$$

This number p is the number of holes involved in the transfer processes.

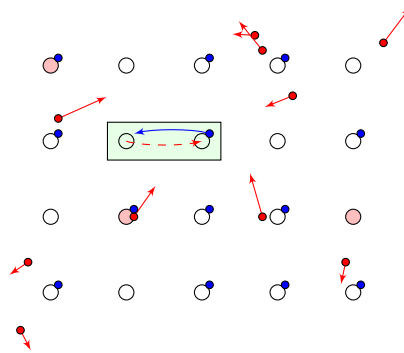
Show that $p \cdot n$ does not depend on the position of the Fermi level E_F . Find the value of $n_i = \sqrt{p \cdot n} \cdot a/L$ for silicon at temperature $T = 300$ K.

A11 What should the Fermi level E_F be so that the crystal is electrically neutral, i.e., the number of holes p is equal to the number of electrons n ?

As we can see, the number of objects involved in the transfer processes depends significantly on the temperature; the edges of the conduction band E_c and the valence band E_v ; and the position of the Fermi level.

Of these three parameters, the position of the Fermi level turns out to be the most interesting, since it can be controlled by impurities:

- By replacing a silicon atom Si in the crystal lattice with an aluminum atom Al, we practically do not change the type of potential $U(x)$ but the number of electrons on the outer shells has decreased by one. That is, the value of $p - n$ has increased by one.
- By replacing a silicon atom Si with phosphorus atom P we practically do not change the form of the potential $U(x)$, but we increase the number of electrons on the outer shells by one. That is, the value of $p - n$ has decreased by one.



Doped silicon in terms of charges then consists of 4 components:

1. Electrically neutral silicon atoms
2. Impurity atoms that are charged $\pm e$ so that their electron shells become the same as those of silicon.
3. Free electrons with negative charge.
4. Positively charged holes that «sit» on the atoms.

The semiconductor as a whole is electrically neutral.

A12 What fraction c of silicon Si atoms must be replaced by aluminum Al to increase the ratio of holes to electrons p/n to $q = 10^6$ with respect to pure silicon? Consider the temperature to be 300 K.