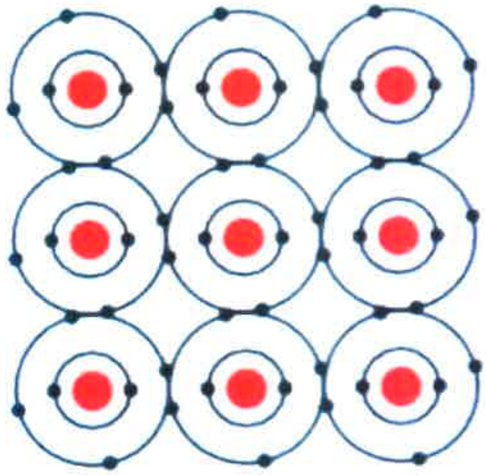
Transport in semiconductors

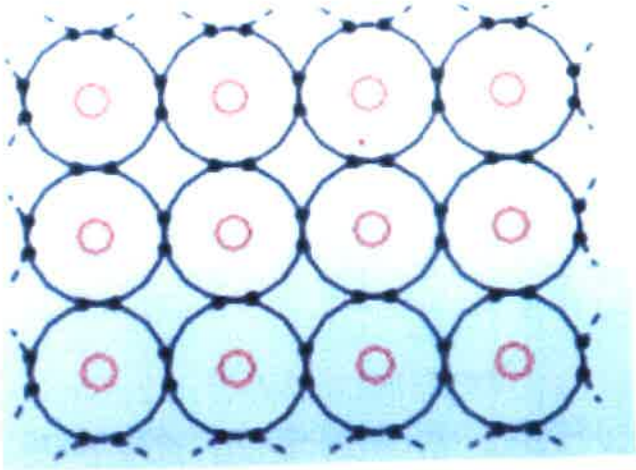
Individual atoms of semiconductors have half-full valence shells. Typical example of a semiconductor is ^{14}Si. It has two electrons in the first shell, 8 electrons in the second shell and 4 electrons in the 3rd - valence shell.

Simplified picture - just the nucleus and valence shell shown

When atoms come together, their share the valence electrons. Therefore, the valence shell is full



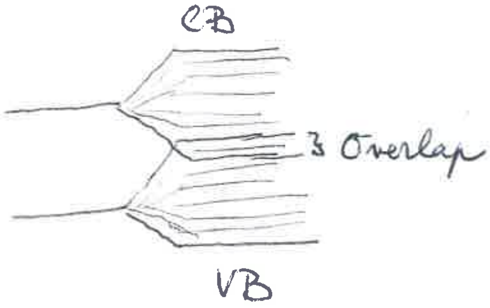
2D projection



Simplified 2D projection

In energy scheme in individual atoms electrons are localized on discrete energy levels. When atoms come together these levels split. If we have N atoms in the solid, from each energy level in individual atom a band consisting of N levels is formed. From the energy state related to the valence shell the valence band (VB) is created. The nearest energy band is called the conduction band. In semiconductors and insulators these two energy bands are separated by an energy interval, where in an ideal periodic structure no electrons can be localized. This bond is called the bandgap. The difference between semiconductors and insulators is in the value of the bandgap. Semiconductors are often defined as materials with energy bandgap ($E_g < 5eV$). Insulators have $E_g > 5eV$. This value is connected with the energy necessary to free electron from the valence shell (transition from VB to CB). It is much smaller in semiconductors than in insulators. The number of electrons that are free at 300K in insulators is small, the electric conductivity is very low.

In metals the valence band and conduction band overlap. There is no bandgap



Examples - Au, Ag, Cu

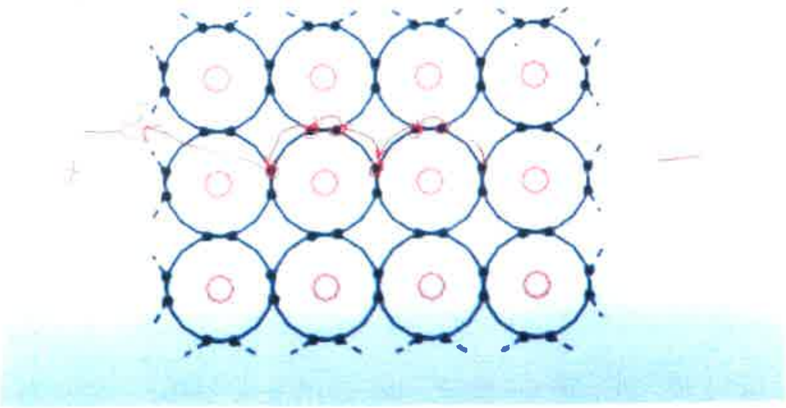
Electrons from the top of the valence band can move freely in the conduction band

Therefore these materials are good conductors.

Intrinsic semiconductors

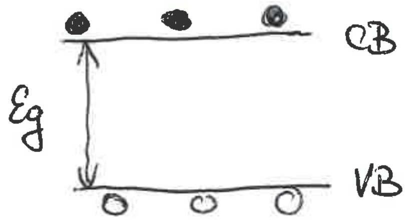
At T=0K all electrons are in the valence shells (Energetically in the valence band). After some increase of temperature there is enough energy (thermal) to free electron from the VB.

Conduction in Intrinsic Semiconductor



An empty state is formed on the original position of the electron. If external bias is applied, the free electron drifts to the anode.

Neighbour electron in the valence shell can transfer to the empty space (hole), creates a new hole, to which another electron can transfer. This way electrons in the valence shells also drift to the anode. This flow can be seen as a flow the holes in the valence band to the anode (hole = missing electron and is therefore positively charged.



In intrinsic semiconductors the electric current is caused by drift of equal numbers of electrons and holes

$n = p$

Doped semiconductors

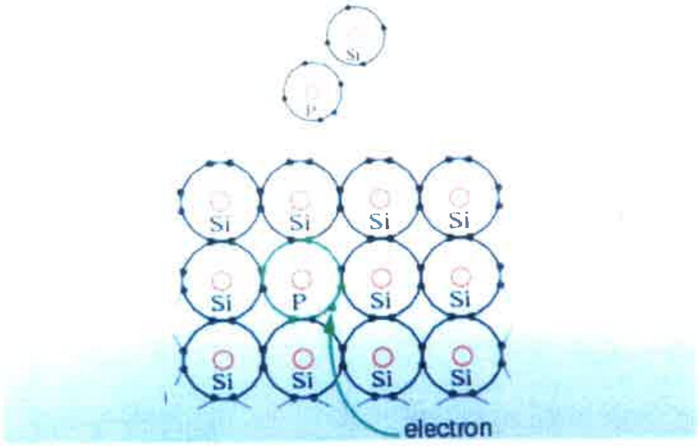
By doping of semiconductors we understand introduction of impurities (other atoms than the atoms of the matrix). The goal of doping is a change of the concentration of free electrons or holes when compared to an intrinsic semiconductor.

If we want to increase the concentration of free electrons we introduce an impurity with a higher number of valence electrons

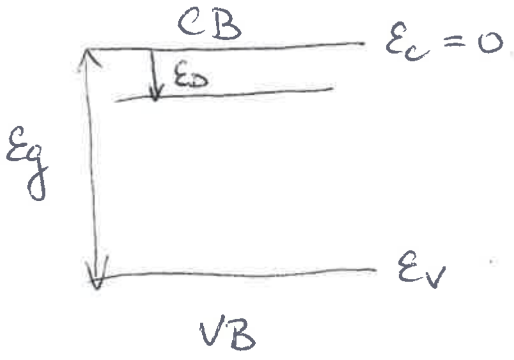
When compared to the matrix. This impurity is called a donor. Example P in Si

P has 5 valence electrons, Si has 4

P



P has a valence electron that is not shared with neighbor atoms. It is weakly bound to nucleus and can be released with a much lower energy than the standard valence electron

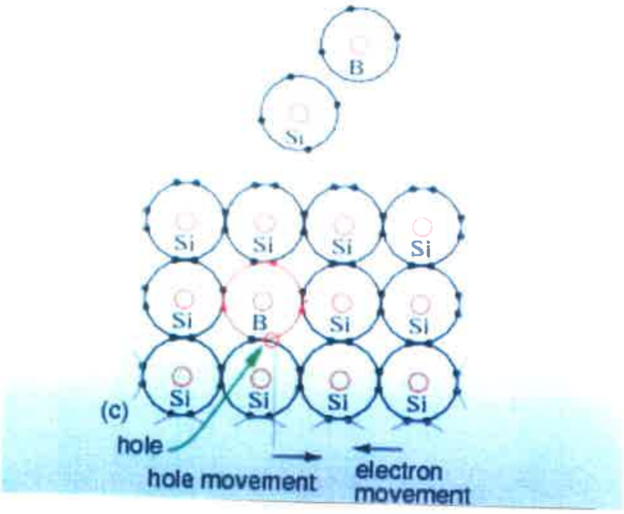


Such an impurity is called „donor"
The semiconductor is called N-type

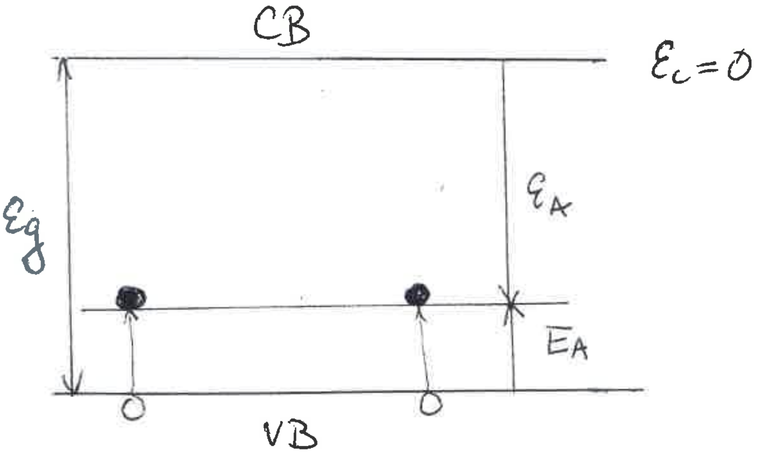
Electrons are so called „majority" carriers, holes are minority carriers.
The electric current is primarily caused by electrons in N-type materials.

If we want to increase the concentration of free holes, we introduce impurity with a smaller number of valence electrons than have the atoms of the matrix.

Example B in Si



Holes formed due to acceptor doping drift after application of bios to the anode.

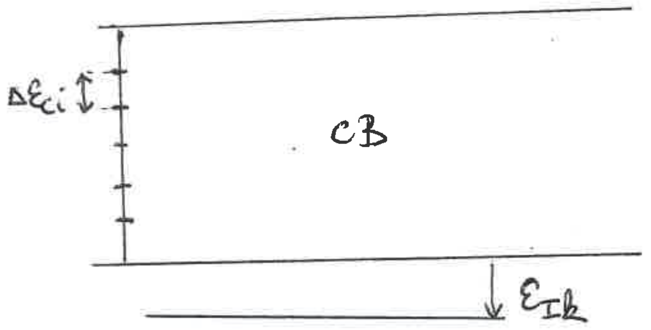


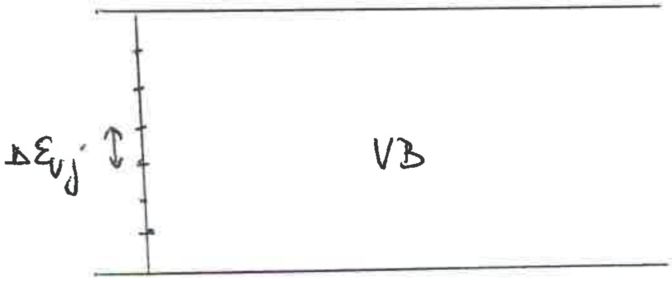
● an electron on acceptor is often symbolized as $\boxed{-}$ .. fixed negative charge on acceptor

Statistics of electrons and holes

Electrons behave like indistinguishable charged particles. Their distribution is described by Fermi distribution function.

To determine the distribution of electrons in the crystals we will be looking for a number of permutations to divide a certain number of electrons to the allowed energy states. These states can be in the bands (described by quantum numbers k_x, k_y, k_z or in the bandgap (caused by impurities or native defects like vacancies, interstitials, antisites etc.) characterized by their own quantum numbers.





Let at given thermodynamic conditions be m_e electrons in the crystal

$$m_e = m_{ce} + m_{ve} + m_{Ie}$$

Here m_{ce} is the number (or concentration) of electrons in the conduction band, m_{ve} is the concentration of electrons in the valence band and m_{Ie} is the concentration of electrons on impurities.

For the purpose of the derivation we divide the conduction band (CB) to energy intervals $\Delta\mathcal{E}_c$ and the valence band (VB) to $\Delta\mathcal{E}_v$. Each interval contains a large number of energy states, but $\Delta\mathcal{E}_{c,v} \ll \Delta\mathcal{E}_H$, where $\Delta\mathcal{E}_H$ characterizes the precision of measurements. Let the i-th interval in the CB contain m_{ci} electrons and N_{ci} states.

The number of permutations how to divide m_{ci} electrons into N_{ci} states is

$$W_{ci} = \binom{N_{ci}}{m_{ci}} = \frac{N_{ci}!}{m_{ci}!\,(N_{ci}-m_{ci})!}$$

The number of permutations how to divide all electrons in the CB is

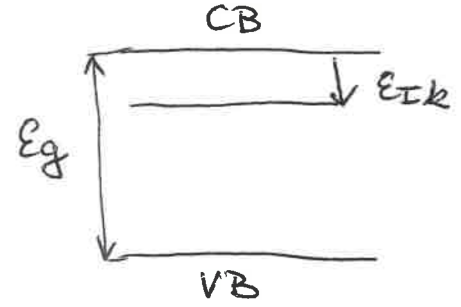
$$W_e = \prod_i W_{ci}$$

The same applies for the valence band

$$W_{v_j} = \frac{N_{v_j}!}{M_{v_j}!\,(N_{v_j}-M_{v_j})!} \qquad W_v = \prod_j W_{v_j}$$

When introducing impurities to statistics we will assume a simple case, when each impurity has just one energy state in the bandgap. It means that if we have a concrete atom with n_a+1 electrons, it is necessary to provide energy ε_{Ik} (k is an index of impurity type) to excite one electron ($\varepsilon_{Ik} < \varepsilon_g$)

Example - a donor (like P in Si)



P has 5 electrons in the valence shell in the ground state (i.e. $n_a+1 = 5$)

After excitation of one electron by energy ε_{Ik} the donor (here P) is ionized, there are 4 electrons in the valence shell.

If the atom is in the state with n_a electrons, energy higher than ε_g is necessary to ionize it further. Therefore, the next energy state of the impurity is in the conduction band.

The number of permutations, how to divide $M_{I\ell}$ electrons into $N_{I\ell}$ states (each atom has one energy state in the energy gap) of the ℓ-th impurity is

$$\binom{N_{Ik}}{M_{I\ell}} = \frac{N_{I\ell}!}{M_{I\ell}!\,(N_{Ik}-M_{Ik})!}$$

$N_{I\ell}$ .. the total number of atoms of the impurity

$M_{I\ell}$ ... the number of atoms with M_a+1 electrons

$N_{I\ell}-M_{I\ell}$ .. the number of atoms with M_a electrons

In case of impurities we have to take into account that electrons can be on each atom in several energetically equal states. For example, if we have three electrons in an orbital that contains 6 states (p-orbital) we have additional

$$g = \binom{6}{3} = \frac{6!}{3!\,3!} = 20$$

The number g is called degeneracy factor

Let g_1 be the degeneracy of the state with M_a+1 electrons and g_0 of the state with M_a electrons.

Then the total number of permutations on all atoms with M_a+1 electrons is

$$(\underbrace{g_1 \cdot g_1 \cdots g_1}_{M_{Ik}}) = g_1^{M_{Ik}}$$

The total number of additional permutations on all atoms with M_a electrons is

$$(\underbrace{g_0 \cdot g_0 \cdots g_0}_{N_{Ik}-M_{Ik}}) = g_0^{N_{Ik}-M_{Ik}}$$

The total number of permutations of electrons on k-th impurity is

$$W_{Ik} = \frac{(g_1)^{M_{Ik}} \cdot g_0^{(N_{Ik}-M_{Ik})} \cdot N_{Ik}!}{M_{Ik}!\,(N_{Ik}-M_{Ik})!}$$

If we have more impurity types in the crystal, then

$$W_I = \prod_k W_{Ik}$$

The number of permutations how to divide electrons in the crystal is then

$$W = W_c \cdot W_v \cdot W_I$$

Now we apply an axiom of probability theory saying that if each permutation which results in the same total energy, has an equal probability, then the most probable distribution is that one, that maximizes W.

Therefore, we look for the maximum of W in the calculation. We will take advantage of the Stirling formula $\ln N! = N \ln N - N$.
We will use the fact that both W and ln W are monothonic fuctions (if W has an maximum, ln W has it too.

During the search for a maximum we have to take into account that the total number of electrons in the system Ne and the total energy of all electrons $\mathcal{E}_t$ must be kept.

$$F_1(n) = \sum_i n_{ci} + \sum_j n_{vj} + \sum_k n_{Ik} = n_e$$

$$F_2(n, \varepsilon) = \sum_i n_{ci} \cdot \varepsilon_{ci} + \sum_j n_{vj} \cdot \varepsilon_{vj} + \sum_k n_{Ik} \varepsilon_{Ik} = \mathcal{E}_t$$

We will be looking for maximum of ln W in respect to conduction band electrons, valence band electrons and electrons on impurities respecting the two above written formulas.

Note: The method of bound extrema (Lagrange multipliers)

The method of Lagrange multipliers is a strategy for finding the local maxima and minima of a function subject to equality constraints (i.e. subject to the condition that one or more equations have to be satisfied exactly by the chosen values of the variables.

Let $f, G_1, G_2 .. G_p$ have continuas partial derivations (1.st order) on a set

$M = \{x_1, x_2 \cdots x_{m+p}\}$ $\quad G_i(x) = 0 \quad i = 1 \cdots p$

If the function f has in $x_0 \in M$ a local extremum respective to M, then exist numbers $\lambda_1^0 \cdots \lambda_p^0$ for which holds

$$\frac{\partial f(x_0)}{\partial x_k} - \sum_{j=1}^{p} \lambda_j^0 \cdot \frac{\partial G_i}{\partial x_k}(x_0) = 0$$

Therefore we will use the method of Lagrange multipliers (bound esctrema) which results in

$$\frac{\partial}{\partial m_a}\left\{ \ln W + \alpha\,(\overbrace{N_e - F_1(m)}^{G_1}) + \beta\,(\overbrace{\mathcal{E}_t - F_2(m,\mathcal{E})}^{G_2}) \right\}$$

where $m_a = m_{ci}$ or m_{vj} or $m_{I\ell}$

So we perform three derivations to look for 3 local maxima (in the CB, VB and on impurities). α and β are the Lagrange multipliers.

Performing the derivations after application of the Stirling formula we obtain

$$m_{ci} = \frac{N_{ci}}{1 + e^{(\alpha + \beta \mathcal{E}_{ci})}}$$

$$m_{vj} = \frac{N_{vj}}{1 + e^{(\alpha + \beta \mathcal{E}_{vj})}}$$

$$m_{I\ell} = \frac{N_{I\ell}}{1 + \frac{g_0}{g_1} e^{(\alpha + \beta \mathcal{E}_{I\ell})}}$$

Based on thermodynamics and statistics it can be determined that

$$\alpha = -\frac{\mathcal{E}_F}{k_B T} \qquad \beta = \frac{1}{k_B T}$$

Derivation of concentration of electrons n_i in the i-th interval of the conduction band

$$\frac{\partial}{\partial n_i} \{ \ln W - \alpha\, G_1(n) - \beta\, G_2(n, \varepsilon) \} = 0$$

$$\ln W = \ln (W_c \cdot W_v \cdot W_I) \,; \quad W_c = \prod_i W_{ci} \,; \quad W_v = \prod_j W_{vj} \quad W_I = \prod_k W_{Ik}$$

$$\ln W = \sum_i \ln W_{ci} + \sum_j \ln W_{vj} + \sum_k \ln W_{Ik}$$

$$\ln W = \sum_i \ln \frac{N_{ci}!}{n_{ci}!\,(N_{ci} - n_{ci})!} + \sum_j \ln \frac{N_{vj}!}{n_{vj}!\,(N_{vj} - n_{vj})!} +$$

$$+ \sum_k \ln \frac{g_1^{\,n_{Ik}} \cdot g_0^{\,N_{Ik} - n_{Ik}} \cdot N_{Ik}!}{n_{Ik}!\,(N_{Ik} - n_{Ik})!} =$$

$$= \sum_i \ln N_{ci}! - \sum_i \ln n_{ci}! - \sum_i \ln (N_{ci} - n_{ci})! + \sum_j (\quad) + \sum_k (\quad)$$

We apply stirling formula

$$\ln A! \approx A \ln A - A$$

$$\frac{\partial \ln W}{\partial n_{ci}} = \frac{\partial}{\partial n_{ci}} \Big(\sum_i N_{ci} \ln N_{ci} - \sum_i N_{ci} - \sum_i n_{ci} \ln n_{ci} + \sum_i n_{ci} -$$

$$- \sum_i (N_{ci} - n_{ci}) \ln (N_{ci} - n_{ci}) + \sum_i (N_{ci} - n_{ci}) \Big\} =$$

$$-1 - \ln n_{ci} + 1 - \frac{N_{ci}}{N_{ci} - n_{ci}} + \frac{n_{ci}}{N_{ci} - n_{ci}} + \ln (N_{ci} - n_{ci}) - 1 =$$

$$= - \ln n_{ci} + \ln (N_{ci} - n_{ci})$$

$$\frac{\partial}{\partial n_i}\{\ln W - \alpha G_1(n) - \beta G_2(n,\varepsilon)\} = 0$$

$$= -\ln n_{ci} + \ln(N_c - n_{ci}) - \alpha - \beta\varepsilon_{ci} = 0$$

(Because $G_1(n) = \sum_i n_{ci} + \sum_j n_{vj} + \sum_k n_{Ik} - n_e$

$$\frac{\partial G_1}{\partial n_{ci}} = 1 \quad ; \text{ etc }\Big)$$

$$\ln\frac{n_{ci}}{N_{ci}-n_{ci}} = -\alpha - \beta\varepsilon_{ci}$$

$$\frac{n_{ci}}{N_{ci}-n_{ci}} = e^{-(\alpha+\beta\varepsilon_{ci})}$$

$$n_{ci} = N_{ci}\cdot e^{-(\alpha+\beta\varepsilon_{ci})} - n_{ci}\cdot e^{-(\alpha+\beta\varepsilon_{ci})}$$

$$n_{ci}\left(1+e^{-(\alpha+\beta\varepsilon_{ci})}\right) = N_{ci}\cdot e^{-(\alpha+\beta\varepsilon_{ci})}$$

$$n_{ci} = \frac{N_{ci}}{1+e^{+(\alpha+\beta\varepsilon_{ci})}}$$

Based on comparison of thermodynamics and statistical physics it can be shown that

$$\alpha = -\frac{\varepsilon_F}{kT} \qquad \beta = \frac{1}{kT}$$

$$\Rightarrow n_{ci} = \frac{N_{ci}}{1+e^{\frac{\varepsilon_{ci}-\varepsilon_F}{kT}}}$$

Statistics of a monovalent donor

I. Neutral (not ionized) donor

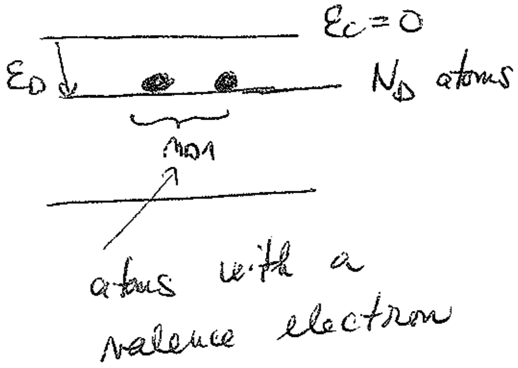
$$M_{D1} = \frac{N_D}{1+\frac{g_0}{g_1}e^{\frac{\varepsilon_D-\varepsilon_F}{k_BT}}}$$

↗ 1 electron on donor

$$g_0 = \binom{2}{0} = \frac{2!}{0!\,2!} = 1$$

$$g_1 = \binom{2}{1} = \frac{2!}{1!\,1!} = 2$$

$$M_{D1} = \frac{N_D}{1+\frac{g_0}{g_1}e^{\frac{\varepsilon_D-\varepsilon_F}{k_BT}}}$$



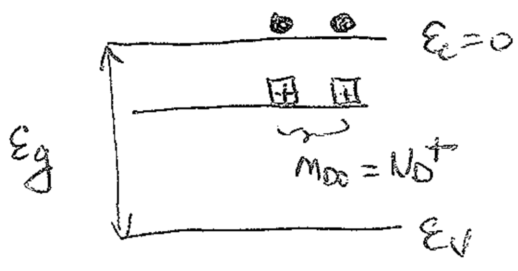
II ionized donor

$$M_{D0} = N_D^+ = N_D - M_{D1} =$$

↗ no electron on donor

$$= N_D - \frac{N_D}{1+\frac{g_0}{g_1}e^{\frac{\varepsilon_D-\varepsilon_F}{k_BT}}} = \frac{N_D}{1+\frac{g_1}{g_0}e^{-\frac{(\varepsilon_D-\varepsilon_F)}{k_BT}}}$$

$$N_D^+ = \frac{N_D}{1+2e^{\frac{-\varepsilon_D+\varepsilon_F}{k_BT}}}$$



Calculation of concentration of electrons in the conduction band

From the previous statistical calculation follows that the concentration of electrons in the i-th energy interval of the CB is

$$n_{ci} = \frac{N_{ci}}{1+e^{\frac{\mathcal{E}_i - \mathcal{E}_F}{k_B T}}}$$

(we set simply) $\mathcal{E}_{ci} = \mathcal{E}_i$

The total number of electrons can be calculated as

$$n = \sum_i n_{ci} = \sum_i \frac{N_{ci}}{1+e^{\frac{\mathcal{E}_i - \mathcal{E}_F}{k_B T}}}$$

Instead of summing all the energy intervals we can use integration. The number of states in the i-th interval N_{ci} is replaced by $g(\mathcal{E}) \cdot \Delta\mathcal{E}_{ci}$ (or $\rho(\mathcal{E})\, d\mathcal{E}$, when $\Delta\mathcal{E}_{ci} \to d\mathcal{E}$

From the theory of semiconductors we know that

$$g(\mathcal{E}) = \frac{4\pi\,(2m_e^*)^{3/2}\sqrt{\mathcal{E}}}{h^3}$$

(in 3D space)

The function $g(\mathcal{E})$ is called the density of states in the energy space.

Then

$$n = \int_{\varepsilon_{CMIN}}^{\varepsilon_{CMAX}} \frac{g(\varepsilon)\,d\varepsilon}{1+e^{\frac{\varepsilon-\varepsilon_F}{kT}}} = \int_{\varepsilon_{CMIN}}^{\varepsilon_{CMAX}} f_0(\varepsilon)\,g(\varepsilon)\,d\varepsilon$$

As we decided to set $\varepsilon_{CMIN} = 0$ and due to the fact that the Fermi-Dirac distribution function $\to 0$ for high ε, we can set $\varepsilon_{CMAX} = \infty$ in the integral to simplify the calculation. Then

$$n = \int_0^{\infty} \frac{g(\varepsilon)\,d\varepsilon}{1+e^{\frac{\varepsilon-\varepsilon_F}{k_BT}}} \quad ; \quad x = \frac{\varepsilon}{kT} \; ; \; \varepsilon = kTx$$

$$d\varepsilon = kT\,dx$$

$$\eta = \frac{\varepsilon_F}{kT}$$

$$n = \frac{4\pi\,(2m_e^*)^{3/2}}{h^3} \int_0^{\infty} \frac{\sqrt{\varepsilon}\,d\varepsilon}{1+e^{\frac{\varepsilon-\varepsilon_F}{k_BT}}} =$$

$$= \frac{4\pi\,(2m_e^* k_BT)^{3/2}}{h^3} \int_0^{\infty} \frac{x^{1/2}\,dx}{1+e^{x-\eta}} =$$

$$= \frac{4\,(2\pi\, m_e^* k_BT)^{3/2}}{\sqrt{\pi}\; h^3} \int_0^{\infty} \frac{x^{1/2}\,dx}{1+e^{x-\eta}}$$

We introduce effective density of states in the CB

$$N_c = \frac{2\,(2\pi\, m_e^* k_BT)^{3/2}}{h^3}$$

Then we obtain

$$n = \frac{2}{\sqrt{\pi}} N_c \int_0^\infty \frac{x^{1/2}\,dx}{1+e^{x-\eta}}$$

This result can be rewritten with the help of the Fermi integral

$$F_r^*(\eta) = \int_0^\infty \frac{x^r}{e^{x-\eta}+1}$$

$$n = \frac{2}{\sqrt{\pi}} N_c F_{1/2}^*(\eta)$$

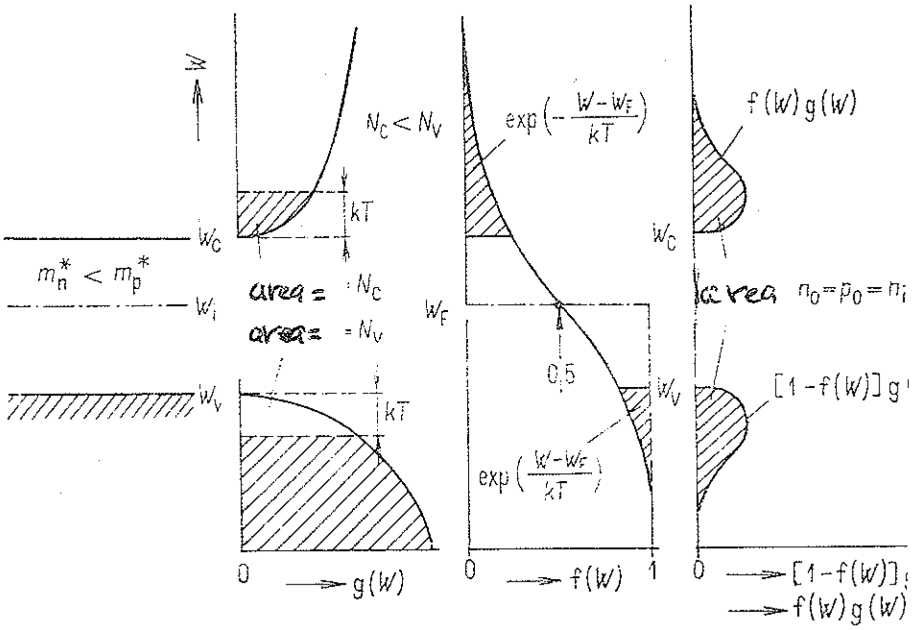
For $\eta < -4$ (i.e. for energies farther than $4kT$ from the bottom of the CB) simplify as

$$F_{1/2}^*(\eta) \approx \frac{\sqrt{\pi}}{2} e^{\eta}$$

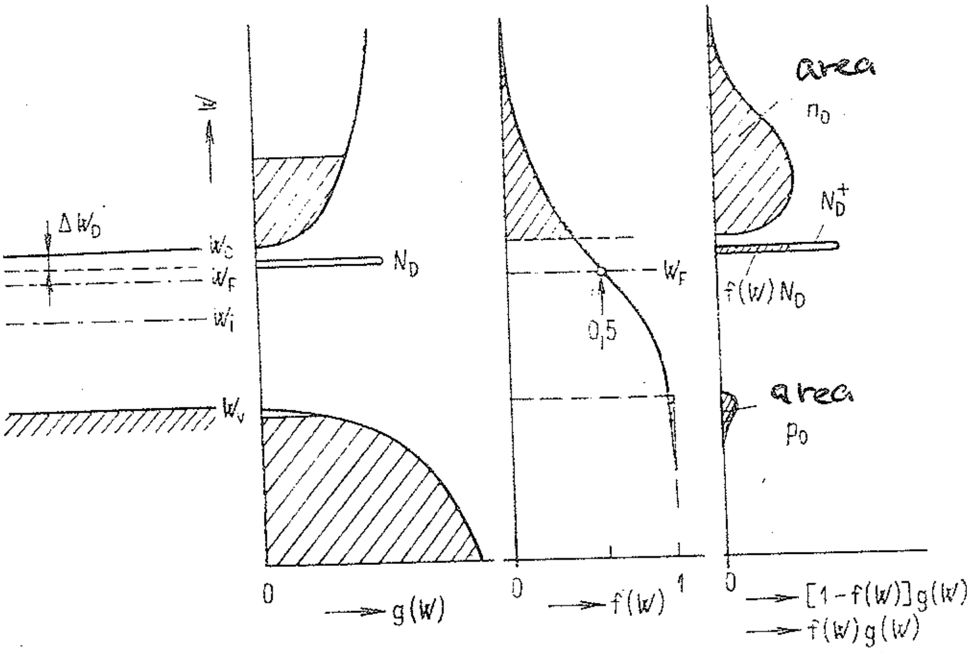
For this so called not degenerate state we can then write

$$n = \frac{2}{\sqrt{\pi}} \cdot \frac{\sqrt{\pi}}{2} N_c e^{\eta} = N_c e^{\eta}$$

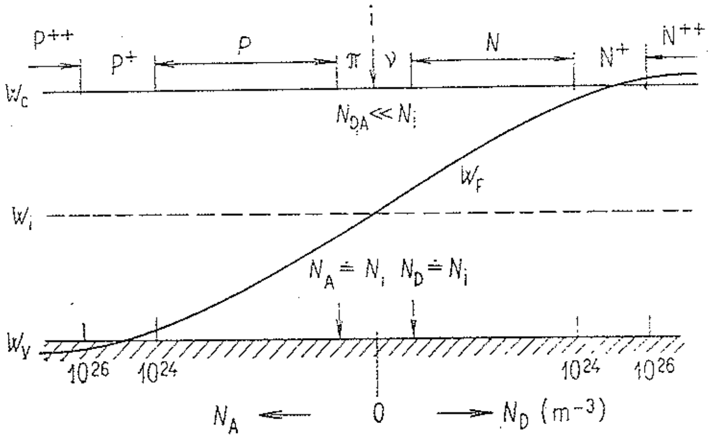
Energies marked as W (instead of E) in these diagrams



a) b) c) d)



a) b) c) d)



Statistics of holes

The distribution function of holes is

$$f_{0,h} = 1 - f_{0,e} = 1 - \frac{1}{1+e^{x-\eta}} = \frac{1}{1+e^{-(x-\eta)}}$$

For a description of statistics for holes we introduce new variables in such a way that equations for holes look like eqs. for electrons.

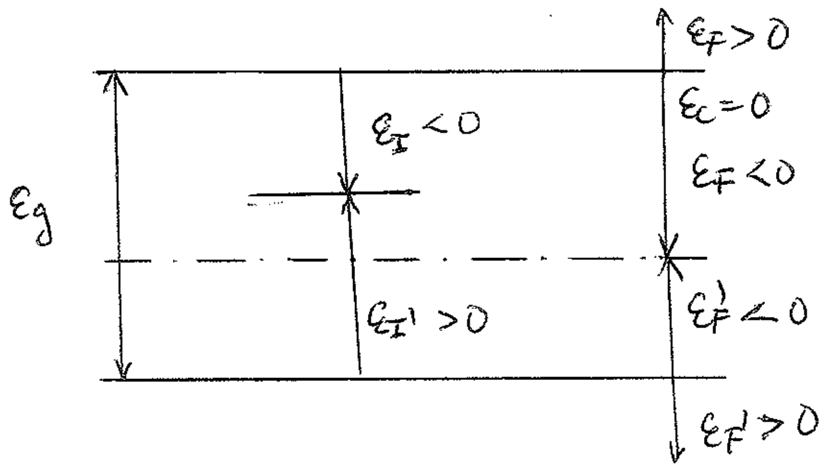
$$\varepsilon' = -\varepsilon - \varepsilon_g \qquad \varepsilon_F' = -\varepsilon_F - \varepsilon_g \ ; \ x' = -x - \beta_g$$

$$\eta' = -\eta - \beta_g$$

$$\left(\eta = \frac{\varepsilon_F}{k_BT},\ \eta' = \frac{\varepsilon_F'}{k_BT};\ \beta_g = \frac{\varepsilon_g}{k_BT},\ x' = \frac{\varepsilon'}{k_BT},\ x = \frac{\varepsilon}{k_BT} \right)$$

$$f_{0,h} = \frac{1}{1+e^{-(x-\eta)}} = \frac{1}{1+e^{-x+\eta}} =$$

$$= \frac{1}{1+e^{x'+\beta_g-\eta'-\beta_g}} = \frac{1}{1+e^{x'-\eta'}}$$



By the same approach that we used to calculate n, we obtain for p

$$p = \int_0^{\infty} f_0(\mathcal{E}')\, g(\mathcal{E}')\, d\mathcal{E}' = \frac{2}{\sqrt{\pi}} N_c\, F_{1/2}(\eta')$$

Here N_v is the effective density of states in the valence band

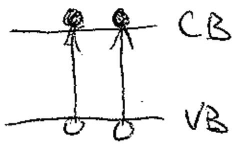
$$N_V = \frac{2(2\pi m_e^* k_B T)^{3/2}}{h^3}$$

$$p = N_v e^{\eta'} \qquad \text{(non-degenerate stat)}$$

Determination of the Fermi energy

1) Intrinsic semiconductor

$n = p$



Electrons in CB come from VB

$$\Downarrow \quad N_c e^{\eta} = N_v e^{\eta'}$$

$$\frac{2(2\pi m_e^* k_B T)^{3/2}}{h^3} e^{\eta} = \frac{2(2\pi m_h^* k_B T)^{3/2}}{h^3} e^{\eta'}$$

$$m_e^{*3/2} e^{\eta} = m_h^{*3/2} e^{\eta'} = m_h^{*3/2} e^{-\eta-\beta g}$$

$$e^{2\eta} = \left(\frac{m_h^*}{m_e^*}\right)^{3/2} e^{-\beta g}$$

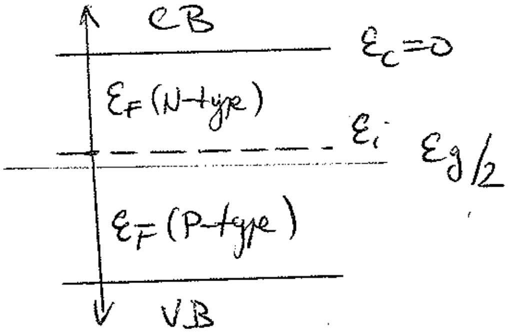
$$\eta = \eta_i = -\frac{\beta g}{2} + \frac{3}{4}\ln\frac{m_h^*}{m_e^*} = -\frac{\varepsilon_g}{2k_BT} + \frac{3}{4}\ln\frac{m_h^*}{m_e^*}$$

The Fermi energy in an intrinsic semiconductor is located slightly above the middle of the bandgap (because $m_h^* > m_e^*$)

Definition of N-type and P-type semiconductor

N-type .. ε_F closer to CB than ε_i (η_F closer than η_i

P-type ε_F closer to VB than ε_i



Intrinsic concentration

$$n_i = n = p$$

$$N_c e^{\eta_i} = N_v e^{-\frac{\beta g}{2}} \cdot \left(\frac{m_h^*}{m_e^*}\right)^{3/4}$$

Let us calculate the product

$$N_c N_v = \frac{2(2\pi m_e^* k_B T)^{3/2}}{h^3} \frac{2(2\pi m_h^* k_B T)^{3/2}}{h^3} (m_e^* m_h^*)^{3/2}$$

$$(N_c N_V)^{1/2} = \frac{2(2\pi k T)^{3/2}}{h^3} \cdot (m_e^* m_h^*)^{3/4} =$$

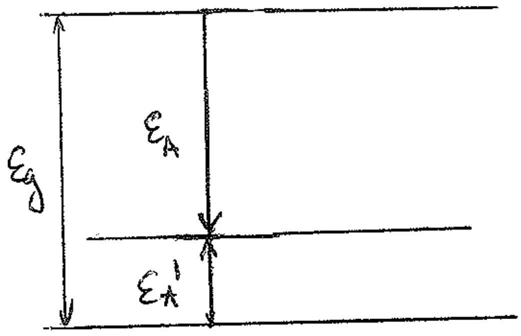
$$= \frac{2(2\pi m_e^* k T)^{3/2}}{h^3} \cdot \left(\frac{m_h^*}{m_e^*}\right)^{3/4} = N_c \left(\frac{m_h^*}{m_e^*}\right)^{3/4}$$

$$\Rightarrow \quad N_c e^{\eta_i} = (N_c N_V)^{1/2} \cdot e^{-\frac{\beta g}{2}} =$$

$$= (N_c N_V)^{1/2} e^{-\frac{\varepsilon_g}{2 k_B T}} = n = p$$

Statistics of a monovalent acceptor

1) Ionized acceptor



$$n_{A1} = \frac{N_A}{1 + \frac{g_0}{g_1} e^{\frac{\varepsilon_A - \varepsilon_F}{k_B T}}}$$

$\varepsilon_A' = -\varepsilon_A - \varepsilon_g$ $\qquad$ $\varepsilon_F' = -\varepsilon_F - \varepsilon_g$

$$n_{A1} = \frac{N_A}{1 + \frac{g_0}{g_1} e^{\frac{-\varepsilon_A' + \varepsilon_F'}{k_B T}}}$$

$$g_0 = \binom{4}{3} = 4$$

$$g_1 = \binom{4}{4} = 1$$

$$n_{A1} = \frac{N_A}{1 + 4 e^{\frac{-\varepsilon_A' + \varepsilon_F'}{k_B T}}} = N_A^+$$

2) Not ionized acceptor

~~N_A~~

$$n_{A0} = N_A - n_{A1} = \frac{N_A}{1 + \frac{1}{4} e^{\frac{\varepsilon_A' - \varepsilon_F'}{k_B T}}}$$

Electric neutrality equation

$$\sum(+) = \sum(-)$$

$$p + N_D^+ = n + N_A^-$$

$$N_D^+ \equiv n_{D0}$$

$$N_A^- \equiv n_{A1}$$

$$n_{D0} = \frac{N_D}{1+2e\,e^{-\varepsilon_d^* + \eta}} \qquad \varepsilon_d^* = \frac{\varepsilon_d}{k_B T} \qquad \eta = \frac{\varepsilon_F}{k_B T}$$

$$n_{A1} = \frac{N_A}{1+4e^{-\varepsilon_A^{*\prime}+\eta'}} \qquad \varepsilon_A^{*\prime} = \frac{\varepsilon_A'}{k_B T} \qquad \eta' = \frac{\varepsilon_F'}{k_B T}$$

$n = N_c e^{\eta}$ (non-degenerate state)

$n = \frac{2}{\sqrt{\pi}} N_c F_{1/2}^*(\eta)$ General form

$$N_c e^{\eta} + \frac{N_D}{1+2e^{-\varepsilon_d^*+\eta}} = N_v e^{\eta'} + \frac{N_A}{1+4e^{-\varepsilon_A^{*\prime}+\eta'}}$$

The solution of ENE for one type of impurities

Let us focus on the case $N_D \neq 0$, $N_A = 0$. We will assume that the temperature T is so low that transitions of electrons from the VB to CB is negligible (i.e. $p=0$)

Then the ENE has a simple form

$$n = N_D^+ \qquad (N_D^+ \equiv n_{D0})$$

$$N_c e^{\eta} = \frac{N_D}{1 + 2e^{-\varepsilon_d^* + \eta}}$$

$$N_c e^{\eta} + 2N_c e^{\eta} e^{-\varepsilon_d^* + \eta} - N_D = 0 \qquad ; \quad e^{\eta} = x$$

$$2N_c e^{-\varepsilon_d^*} x^2 + N_c x - N_D = 0$$

$$D = N_c^2 + 8 N_c N_D e^{-\varepsilon_d^*}$$

$$x = \frac{1}{4}\left(\sqrt{1 + 8\frac{N_D}{N_c} e^{-\varepsilon_d^*}} - 1\right) e^{\varepsilon_d^*}$$

$$\varepsilon_d^* < 0 \Rightarrow -\varepsilon_d^* > 0$$

when $T \to 0$ $\qquad 8\frac{N_D}{N_c} e^{-\varepsilon_d^*} \gg 1 \Rightarrow$

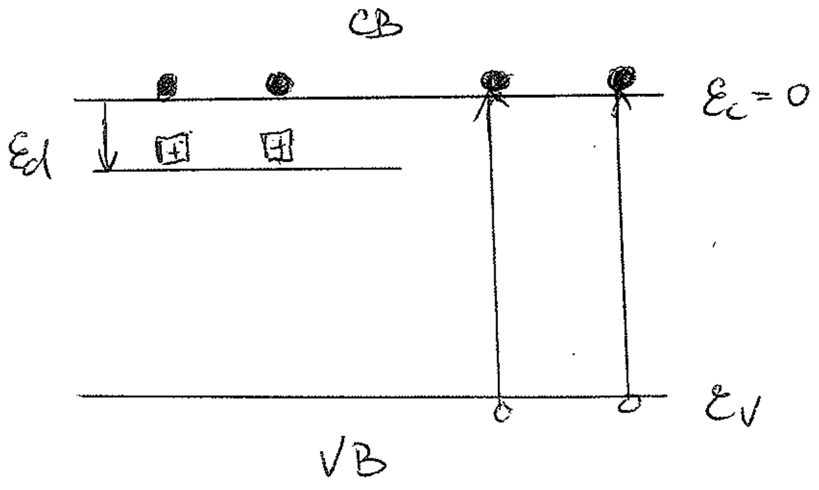
$$\sqrt{\frac{N_D}{2N_c}}\, e^{-\frac{\varepsilon_d^*}{2}} e^{\varepsilon_d^*} = e^{\eta}$$

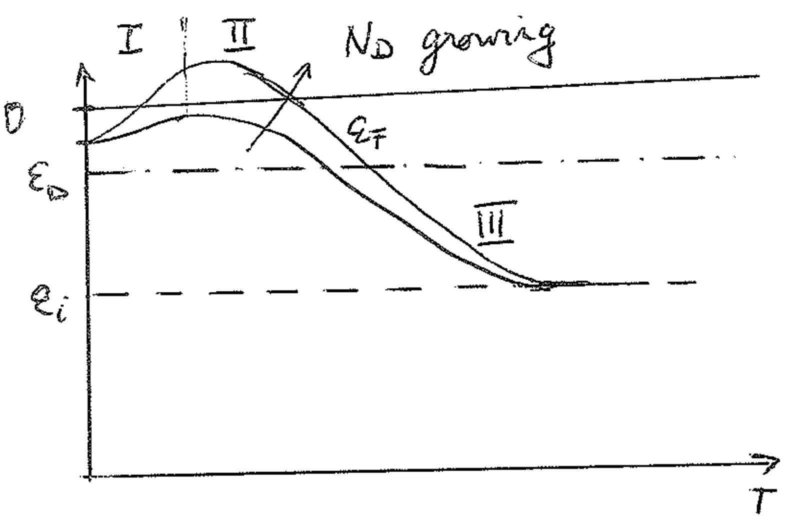
$$\Rightarrow \eta = \frac{\varepsilon_d^*}{2} + \frac{1}{2}\ln\frac{N_D}{2N_c} \; (*) \; ; \quad \varepsilon_F = \frac{\varepsilon_d}{2} + \frac{1}{2}k_B T \ln\frac{N_D}{2N_c}$$

It follows from the result that at $T=0$ the Fermi energy is in the middle of the energy level of the donor and the bottom of the CB

The course of $\varepsilon_F(T)$ is described by equation (+) to the temperature, when transcitions of electrons from the VB to the CB start to contribute and the ENE has a more complex form

$$n = N_D^+ + p \qquad (++)$$





With an increasing temperature in region I the ε_F is shifting from its position at $T=0$ ($\varepsilon_D/2$) towards the CB. When transitions of electrons from the VB to CB start to be significant, holes are generated, too. This leads to the fact, that the $\varepsilon_F(T)$ reaches a maximum and starts to shift down towards the middle of the bandgap. Finally it reaches the intrinsic Fermi energy ε_i. In this situation, the concentration of electrons in the CB coming from donors is negligible when compared to concentration of electrons coming from the CB (i.e $n \approx p$).

The situation for acceptors is treated analogically.

$$\varepsilon_F' = \frac{\varepsilon_A'}{2} + \frac{k_B T}{2} \ln \frac{N_A}{2N_V}$$

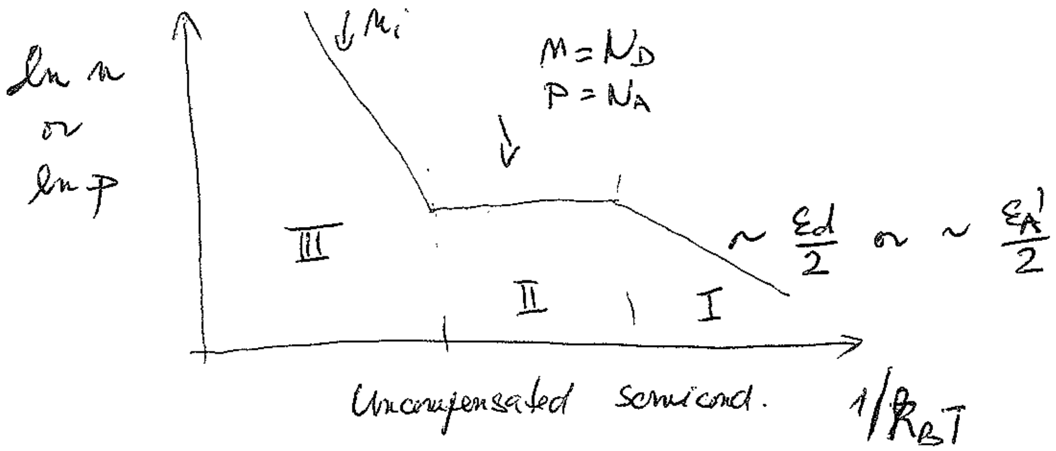
Where ε_F', ε_A' is calculated from the top of VB, N_V is effective density of states in VB.

The solution of ENE in a general form is possible only numerically

The solution yields Fermi energy and concentration of free carriers

Uncompensated semiconductor:

Dependence of $n(T)$ - or $p(T)$



Region I ... low temperatures

$$\varepsilon_F = \frac{\varepsilon_D}{2} + \frac{k_BT}{2} \ln \frac{N_D}{2N_c} \quad \left(\eta = \frac{\varepsilon_d^*}{2} + \frac{1}{2} \ln \frac{N_D}{2N_c} \right)$$

or

$$\varepsilon_F' = \frac{\varepsilon_A'}{2} + \frac{k_BT}{2} \ln \frac{N_A}{2N_V} \quad \left(\eta' = \frac{\varepsilon_A'^*}{2} + \frac{1}{2} \ln \frac{N_A}{2N_V} \right)$$

$$\Rightarrow \quad n = \left(\frac{N_D}{2N_c} \right)^{1/2} e^{\varepsilon_d/2k_BT}$$

$$p = \left(\frac{N_A}{2N_V} \right)^{1/2} e^{\varepsilon_A'/2k_BT}$$

Region II - plateau: all electrons from donors are free (in the CB), all donors are ionized. The temperature is too low to enable thermal transitions from VB to CB.

In this interval of T the n remains constant (analogically for p-type semiconductor)

$$n = N_D - N_A \qquad (\text{for } N_D > N_A)$$

or

$$p = N_A - N_D \qquad (\text{for } N_A > N_D)$$

Region III - transitions of electrons from the VB to the CB start to dominate the

$$n = \underbrace{N_D^+}_{\text{negligible}} + p \qquad\qquad p = \underbrace{N_A^-}_{\text{negligible}} + n$$

$$p \gg N_D^+ \qquad\qquad n \gg N_A^-$$

The semiconductor approaches an „intrinsic" state $(n = p)$

According to our previous calculation

$$n = p = N_c e^{\eta_i} = N_c e^{\frac{\varepsilon_{Fi}}{k_BT}} = n_i$$

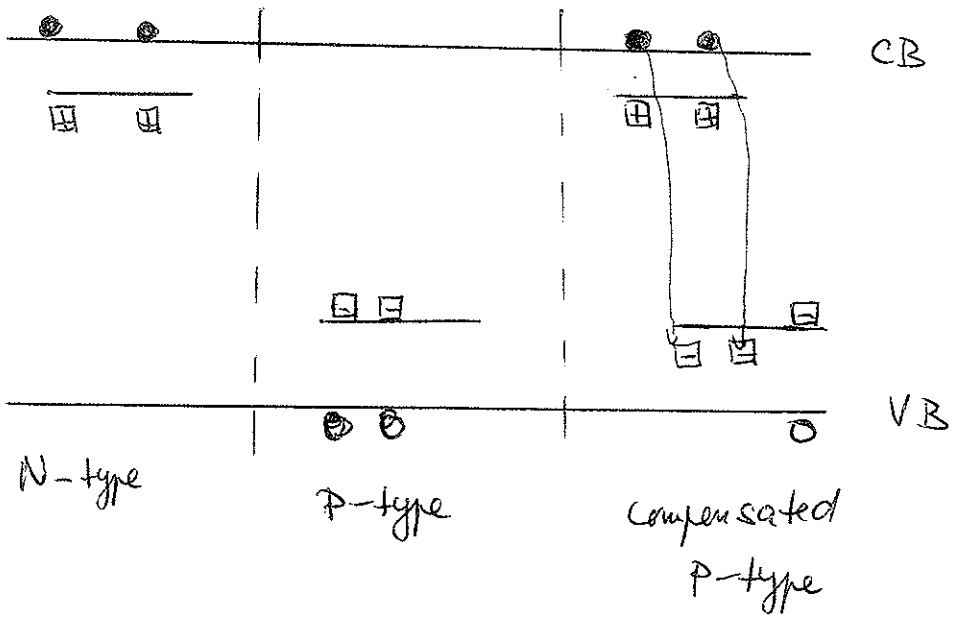
$$\eta_i = -\frac{\varepsilon_g}{2k_BT} + \frac{3}{4}\ln\frac{m_h^*}{m_e^*}$$

$$\Rightarrow \quad n = p = n_i \sim e^{-\frac{\varepsilon_g}{2k_BT}}$$

$$\ln n \sim -\frac{\varepsilon_g}{2k_BT}$$

Compensated semiconductor

The semiconductor is compensated when both donors and acceptors are present in the material



Electrons liberated from donors occupy empty states on acceptors, because these states are energetically more favorable.

If $N_D < N_A$, some atoms of acceptors remain negatively charged and there is a corresponding concentration of free holes in the VB. The semiconductor is P-type, but the concentration of holes is much smaller when compared to uncompensated P-type.

If $N_D > N_A$ the situation is opposite.

Electrons from donors occupy all free sites on acceptors. The remaining electrons in CB cause N-type conductivity of the material.

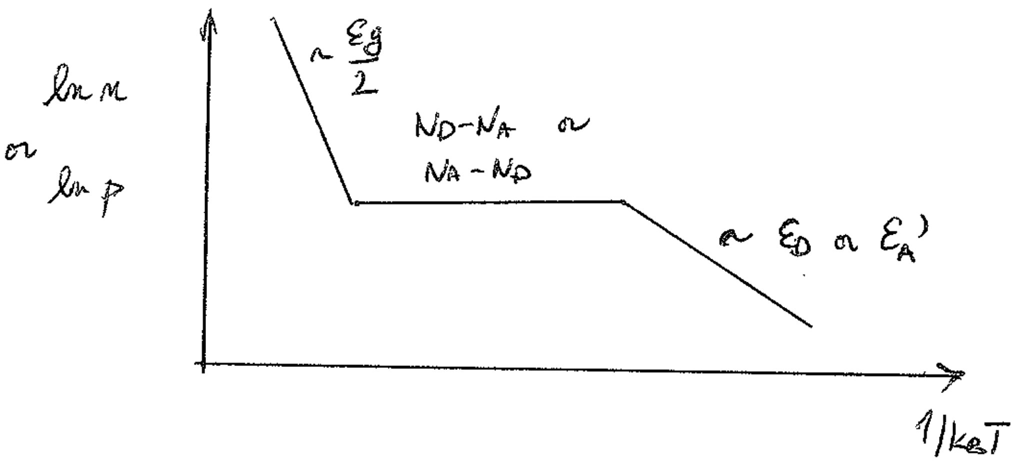
Solution of ENE for compensated semiconductors results in

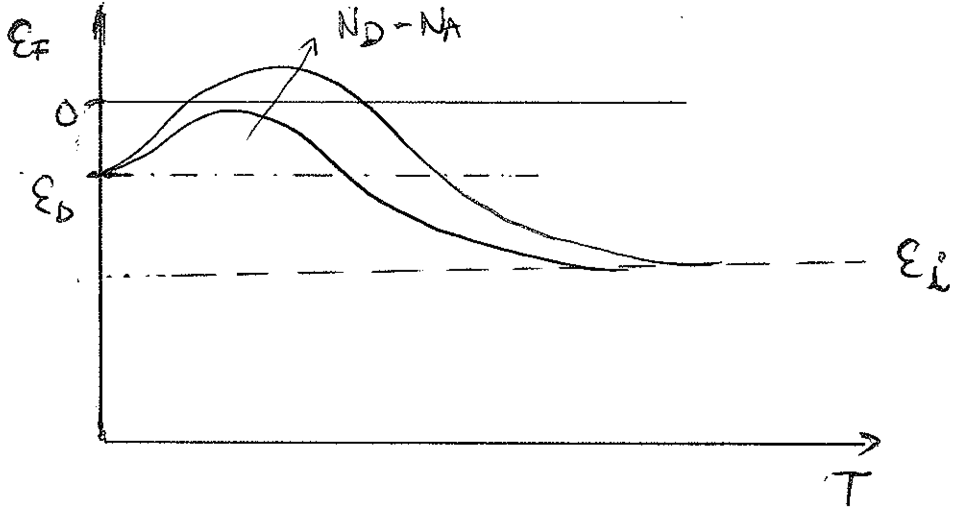
$$\varepsilon_F = \varepsilon_D + \frac{k_B T}{2} \ln \frac{(N_D - N_A)}{2N_C} \qquad \left(\eta = \varepsilon_D^* + \frac{1}{2} \ln \frac{(N_D - N_A)}{2N_C}\right)$$

$$\varepsilon_F' = \varepsilon_A' + \frac{k_B T}{2} \ln \frac{(N_A - N_D)}{2N_V} \qquad \left(\eta = \varepsilon_A'^* + \frac{1}{2} \ln \frac{(N_A - N_D)}{2N_V}\right)$$

$$\Rightarrow \quad n = \left(\frac{N_D - N_A}{2N_C}\right)^{1/2} e^{\varepsilon_D / k_B T}$$

$$p = \left(\frac{N_A - N_D}{2N_V}\right)^{1/2} e^{\varepsilon_A' / k_B T}$$





Compensated N-type semiconductor

Boltzmann transport equation (BTE)

So far we have described a semiconductor in equilibrium. We have used the corresponding equilibrium functions f_0 (f_{0e}, f_{0h} and f_{0k})

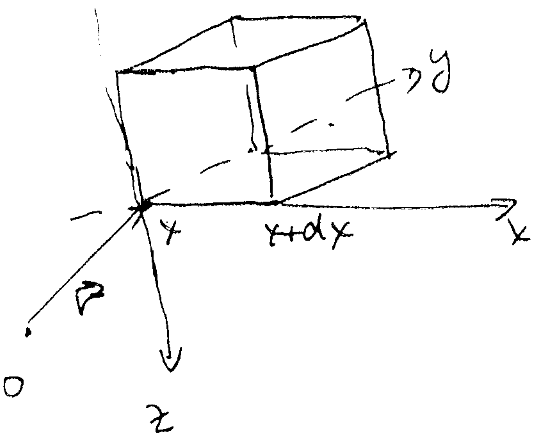
In the next chapters we will deal with non-equilibrium situation, when external fields are applied (bias, temperature gradient, magnetic field ..)

The system of electrons out of equilibrium is described by non-equilibrium distribution function $f(\vec{v}, \vec{r}, t)$.

Number of electrons that are at time t in position $\vec{r}$ (in d^3r elementary volume) and with velocity $\vec{v}$ (in d^3v elementary volume) is

$$f(\vec{v}, \vec{r}, t)\, d^3v\, d^3r$$

Let us now analyse in the $d^3r\, d^3v$ volume of the phase space the change of the number of electrons ΔN. We choose one direction of movement of electrons, e.g. the „x" direction.



$$\Delta N_x = f(\vec{v}, x, y, z, t)\, d^3v\, dx\, dy\, dz - f(\vec{v}, x+dx, y, z, t)\, dx\, dy\, dz$$

Because we study the movement of particle in direction +x with velocity v_x; $dx = v_x dt$

$$\Delta N_x = f(\vec{v}, x, y, z, t)\, d^3v\, v_x\, dt\, dy\, dz - f(\vec{v}, x+dx, y, z, t)\, v_x\, dt\, dy\, dz$$

We multiply this equation by $\frac{dx}{dx}$ and obtain

$$\Delta N_x = \frac{f(\vec{v}, x, y, z, t)\, d^3v\, v_x\, dt\, dx\, dy\, dz - f(\vec{v}, x+dx, y, z, t)\, v_x\, dt\, dx\, dy\, dz}{dx}$$

which means that

$$\Delta N_x = -\frac{\partial f(\vec{v}, x, y, z, t)}{\partial x}\, d^3v\, v_x\, dt\, dx\, dy\, dz$$

The same approach can be applied in y and z directions. In total we have

$$\Delta N_{\vec{r}} = -\left(\frac{\partial f(\vec{v}, x, y, z, t)}{\partial x} v_x + \frac{\partial f(\vec{v}, x, y, z, t)}{\partial y} + \frac{\partial f(\vec{v}, x, y, z, t)}{\partial z} \right) d^3v\, dt\, dx\, dy\, dz$$

We can symbolically write it as

$$\Delta N_{\vec r} = -\vec v \cdot \nabla_{\vec r} f \, d^3v \, d^3r \, dt \quad \text{or}$$

$$\Delta N_{\vec r} = -\vec v \cdot \nabla_{\vec r} f \, d\vec v \, d\vec r \, dt$$

We described a change of number of electrons in the elementary volume $d^3v \, d^3r$ due to the flow in $\vec r$ space.

Electrons can come to or leave the $d^3v \, d^3r$ volume also by change of velocity $\vec v$ (acceleration or deceleration). To describe it we can apply the same approach as in $\vec r$ space and obtain

$$\Delta N_{\vec v} = -\dot{\vec v} \, \nabla_{\vec v} f \, d^3v \, d^3r \, dt = -\vec a \, \nabla_{\vec v} f \, d^3v \, d^3r \, dt$$

$$\Delta N_{tot} = \Delta N_{\vec v} + \Delta N_{\vec r} = -(\vec v \, \nabla_{\vec r} f + \vec a \, \nabla_{\vec v} f) \, d^3v \, d^3r \, dt$$

The total bilance ΔN_{tot} can be described also as a change of a number of electrons in the volume $d^3v \, d^3r$ between times t and $t+dt$.

$$\Delta N_{tot} = \left[f(\vec v, \vec r, t+dt) - f(\vec v, \vec r, t) \right] d^3v \, d^3r$$

We multiply by $\frac{dt}{dt}$ and obtain

$$\Delta N_{tot} = \frac{f(\vec v, \vec r, t+dt) - f(\vec v, \vec r, t)}{dt} \, d^3v \, d^3r \, dt$$

$$\Delta N_{tot} = \frac{\partial f}{\partial t} \, d^3v \, d^3r \, dt$$

Dividing the terms by $d\vec{r}\,d\vec{v}\,dt$ we obtain

$$\frac{\partial f}{\partial t} = \underbrace{-\vec{v}\nabla_{\vec{r}} f - \vec{a}\nabla_{\vec{v}} f}_{\text{the so called „field" term of BTE}}$$

We have now described acting of the external field (potential gradient, magnetic field). To the equation we have to include also scattering of particles. Thanks to scattering there is not a permanent increase of velocity (like in vacuum). In solid state, thanks to scattering, particles will have a constant velocity $\vec{v}_D = \mu\vec{E}$. It is called drift velocity, the constant μ is called „mobility". In order to describe scattering we introduce a quantity

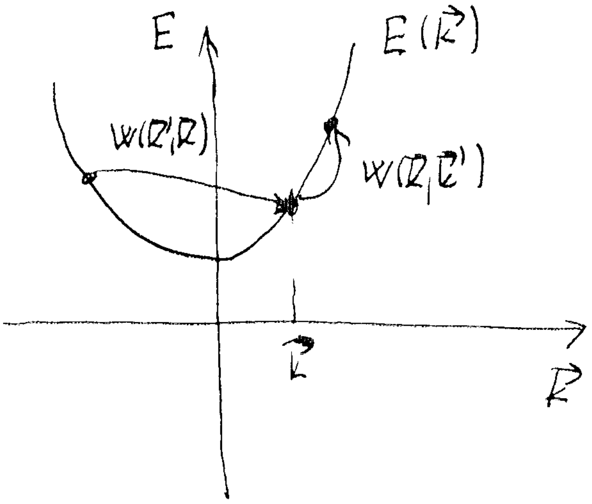
$W(\vec{v},\vec{v}')$ – probability of scattering of electron with velocity $\vec{v}$ to the state with velocity $\vec{v}'$.

This scattering will the total concentration of particles in phase volume $d^3r\,d^3v$ decrease. On the contrary the scattering $\vec{v}' \to \vec{v}$ described by the probability $W(\vec{v}',\vec{v})$ will increase the total number of particles in $d^3r\,d^3v$

When describing transport in solid state we use the quasiimpuls $\vec{p} = \hbar\vec{k}$.

$$\vec{p} = \hbar\vec{k} = m^*\vec{v}$$

Therefore we will further work with probabilities $W(\vec{k},\vec{k}')$ and $W(\vec{k}',\vec{k})$



The intensity of transitions $\vec{k}\to\vec{k}'$ and $\vec{k}'\to\vec{k}$ is not given only by the probability of transitions, but also by occupation of the initial and final states.

The ~~total~~ bilance can be written as

$$\frac{\partial f}{\partial t} = \overbrace{-\vec{v}\nabla_{\vec{r}} f - \vec{a}\nabla_{\vec{v}} f}^{\text{field term}} + \sum_{\vec{k}'} \overbrace{W(\vec{k}',\vec{k}) f(\vec{k}')(1-f(\vec{k})}^{\text{scattering term}} - W(\vec{k},\vec{k}') f(\vec{k})(1-f(\vec{k}')))$$

This is the Boltzmann transport equation (BTE)

Conditions of validity of BTE

- it is a single-particle description
- We use in the description statistical distribution function. This means that there must be a sufficient number of particles in the system
- When describing the distribution we have together the knowledge of position $\vec{r}$ and velocity $\vec{v}$. This corresponds to the classical description

On the contrary the scattering probability W will be described quantum-mechanically. The ΔE can be therefore considered as semi-classical equation

The conditions of validity will be further determined by uncertainty relations

at first we use the relation between the coordinate and the momentum

$\Delta x \cdot \Delta p \gg \frac{\hbar}{2}$. The uncertainty in momentum can be connected to kinetic energy $k T$

$$E = \frac{p^2}{2m} = k_B T$$ (from equipartition teorem $E = \frac{3}{2} k_B T$, but we are interested only in order of magnitude estimate)

$$\Rightarrow \Delta x \gg \frac{\hbar}{2\Delta p} = \frac{\hbar}{2\sqrt{2m k_B T}};$$

here $\lambda_B = \frac{\hbar}{\sqrt{2m k_B T}}$ is the de Broglie wavelength

at $T = 300\ k$ $\lambda_B \approx 10\text{-}20\ nm$ depending on m

This results means that the coordinate (position) of the particle cannot be defined with precision of λ_B. This is equivalent to the requirement that the potential must change slowly relative to λ_B.

Now we will deal with the uncertainty of energy and time

$$\Delta E . \Delta t \gg \frac{\hbar}{2}$$

$E \approx k_B T \Rightarrow \tau \gg \frac{\hbar}{k_B T}$; multiplying by v

we obtain the mean free path

$$\langle l \rangle = \tau \cdot v \gg \frac{\hbar v}{k_B T}$$

The velocity is connected with momentum p

$$v = \frac{p}{m} = \frac{\sqrt{2 m k_B T}}{m}$$

$$\langle l \rangle \gg \frac{\sqrt{2 m k_B T}\,\hbar}{m k_B T} \approx \frac{\hbar}{\sqrt{2 m k_B T}} = \lambda_B$$

it means that the mean free path must be much larger than the de Broglie wavelength

We will again use the relation

$$\Delta E . \Delta t \gg \frac{\hbar}{2} \Rightarrow \Delta t \gg \frac{\hbar}{2 k_B T}$$

and transform the relation to frequency

$$f \approx \frac{1}{\Delta t} \ll \frac{2 k_B T}{\hbar} \approx 10^{12}\,Hz$$

It means that the frequency of changes of conditions in the sample must be smaller than 1THz

Today the electronics typically works in GHz range. This condition is therefore sufficiently fullfiled.

Before we proceed with further analysis of BTE, let us discuss, how to use the result of the solution of BTE, the distribution function f to calculate useful and experimentally measurable physical quantities - like e.g. electric current.

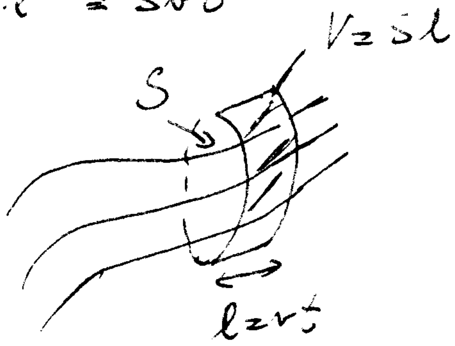
The electric current $I = \frac{Q}{t}$ is the el. charge that passes through area S in time t.

The electric current density $j = \frac{I}{S} = \frac{Q}{St} = \frac{\rho V}{St}$

ρ ... el. charge density
V .. volume of the sample

The electric charge passes in time t the length l. that is connected to velocity v $l = vt$

$V = S \cdot l = Svt$



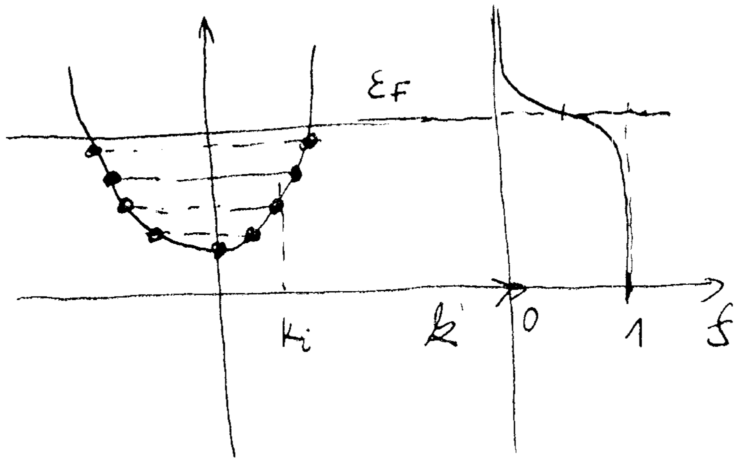
$$\Rightarrow \quad \vec{j} = \rho \frac{Svt}{St} = \rho \vec{v}$$

If we work in the reciprocal state, we can write this equation separately for each state $\vec{k}$:

$$j(\vec{k}) = \rho\, v(\vec{k})$$

The total electric current density is then

$$\vec{j} = \sum_{\vec{k}} j(\vec{k}) = \sum_{\vec{k}} \rho v(\vec{k})$$



Each state can contain 2 electrons (spin)

If the crystal has volume V then

$$\rho(\vec{k}) = -\frac{2e\,f(\vec{k})}{V}$$

$f(\vec{k})$ -- distribution function -- how many electrons are in the k state

We have for the el. current density

$$\vec{j} = \sum_{\vec{k}} \rho v(\vec{k}) = \sum_{\vec{k}} \frac{(-2e)\,f(\vec{k})}{V}\, v(\vec{k})$$

Now in the quasicontinuum we proceed from summation to integration by relation

$$\sum_{\vec{k}} \Rightarrow g_k \int d\vec{k}$$

g_k .. density of states in the $\vec{k}$ - space

$$g_k = \frac{V}{(2\pi)^3}$$ (in the 3D space)

→ will be derived in lecture on solid state physics

$\Downarrow$

$$\vec{j} = \frac{-2e}{(2\pi)^3} \int_{R^3} f(\vec{k})\, v(\vec{k})\, d\vec{k}$$

We will now discuss the relation between probabilities $W(\vec{k},\vec{k}')$ and $W(\vec{k}',\vec{k})$.

We will use the principle of detailed balance. It says that in thermodynamic equilibrium the scattering rates $\vec{k}\to\vec{k}'$ and $\vec{k}'\to\vec{k}$ are equal

$$W(\vec{k},\vec{k}')\, f_0(\vec{k})(1-f_0(\vec{k}')) = W(\vec{k}',\vec{k})\, f_0(\vec{k}')(1-f_0(\vec{k}))$$

$$W(\vec{k},\vec{k}')\cdot \frac{1}{1+e^{\frac{\varepsilon-\varepsilon_F}{k_BT}}}\cdot\left(1-\frac{1}{1+e^{\frac{\varepsilon'-\varepsilon_F}{k_BT}}}\right) = W(\vec{k}',\vec{k})\cdot\frac{1}{1+e^{\frac{\varepsilon'-\varepsilon_F}{k_BT}}}\left(1-\frac{1}{1+e^{\frac{\varepsilon-\varepsilon_F}{k_BT}}}\right)$$

$$W(\vec{k},\vec{k}')\cdot\frac{1}{1+e^{\frac{\varepsilon-\varepsilon_F}{k_BT}}}\cdot\frac{e^{\frac{\varepsilon'-\varepsilon_F}{k_BT}}}{1+e^{\frac{\varepsilon'-\varepsilon_F}{k_BT}}} = W(\vec{k}',\vec{k})\cdot\frac{1}{1+e^{\frac{\varepsilon'-\varepsilon_F}{k_BT}}}\cdot\frac{e^{\frac{\varepsilon-\varepsilon_F}{k_BT}}}{1+e^{\frac{\varepsilon-\varepsilon_F}{k_BT}}}$$

$$\Rightarrow \quad W(\vec{k},\vec{k}')\cdot e^{\frac{\varepsilon'}{k_BT}} = W(\vec{k}',\vec{k})\, e^{\frac{\varepsilon}{k_BT}}$$

We will further deal only with elastic scattering, when $\varepsilon=\varepsilon' \Rightarrow$

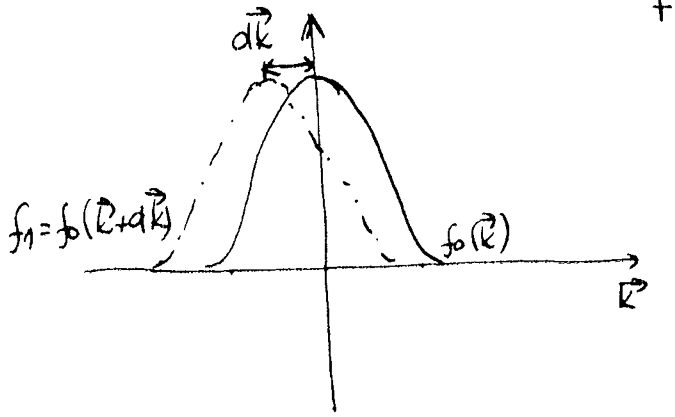
$$W(\vec{k},\vec{k}') = W(\vec{k}',\vec{k})$$

Introduction of relaxation time τ

We will consider only small deviations from equilibrium after application of the external fields. The non-equilibrium distribution function f will be considered in the form

$$f(\vec{k}) = f_0(\vec{k}+\delta\vec{k})$$

This is a shifted Fermi-Dirac distribution



$F \cdot dt = \hbar dk = qEdt$
! electric force

$qEdt = -eEdt = \hbar dk$

$\Rightarrow -dk = \frac{eEdt}{\hbar}$

↗ example of dk when the force is electric field

For small deviations from equilibrium we can approximate $f(\vec{k})$ using Taylor expansion

$$f(\vec{k}) = f_0(\vec{k}) + \nabla_{\vec{k}} f_0(\vec{k}) \cdot d\vec{k} = f_0 + f_1$$

In a parabolic band we have $\mathcal{E} = \frac{\hbar^2 k^2}{2m_e^*}$

$$\nabla_{\vec{k}} f_0 = \frac{\partial f_0}{\partial \mathcal{E}} \cdot \frac{\partial \mathcal{E}}{\partial \vec{k}} = \frac{\partial f_0}{\partial \mathcal{E}} \frac{\hbar^2 \vec{k}}{m_e^*}$$

We can then re-write the scattering term

$$\left(\frac{\partial f}{\partial t}\right)_S = \sum_{\vec{k}'} \left\{ W(k',k) f(\vec{k}')(1-f(\vec{k}) - W(\vec{k},\vec{k}') f(\vec{k})(1-f(\vec{k}')\right\}$$

Taking into account $W(\vec{k},\vec{k}') = W(\vec{k}',\vec{k})$ we obtain

$$\left(\frac{\partial f}{\partial t}\right)_S = \sum_{\vec{k}'} W(\vec{k},\vec{k}')\left(f_1(\vec{k}') - f_1(\vec{k})\right) = -f_1(\vec{k}) \sum_{\vec{k}'} W(\vec{k},\vec{k}')\left(1 - \frac{f_1(\vec{k}')}{f_1(\vec{k})}\right)$$

$= -\frac{f_1(\vec{k})}{\tau}$; where we have introduced the relaxation time τ as

$$\frac{1}{\tau} = \sum_{\vec{k}'} W(\vec{k},\vec{k}')\left(1 - \frac{f_1(\vec{k}')}{f_1(\vec{k})}\right)$$

Physical meaning of relaxation time

$$\left(\frac{\partial f}{\partial t}\right)_S = -\frac{f_1}{\tau} = -\frac{(f-f_0)}{\tau} \quad ; \quad \frac{d(f-f_0)}{(f-f_0)} = -\frac{dt}{\tau}$$

$$\ln(f-f_0) = -\frac{t}{\tau} + \ln C$$

$$t = 0 \qquad \ln(f-f_0)\Big|_{t=0} = \ln C$$

$$\ln\left(\frac{(f-f_0)}{(f-f_0)_{t=0}}\right) = -\frac{t}{\tau}$$

$$(f-f_0) = (f-f_0)_{t=0}\, e^{-\frac{t}{\tau}}$$

When $t=\tau$ $\quad (f-f_0)_\tau = \frac{(f-f_0)_{t=0}}{e}$

$\Rightarrow$ Relaxation time is a time at which deviation from equilibrium drops to 1/e of its initial value

Let us continue with derivation of the formula for relaxation time τ

Taking into account that $f_1(\vec{k}) = \frac{\partial f_0}{\partial \varepsilon} \cdot \frac{\hbar^2 k}{m_e^*}\, d\vec{E}$

we introduce a new function $\vec{\chi} = \frac{\hbar^2}{m_e^*} d\vec{E}$

Then $f_1(\vec{k}) = \left(\frac{\partial f_0}{\partial \varepsilon}\right) \vec{\chi}\cdot\vec{k}$

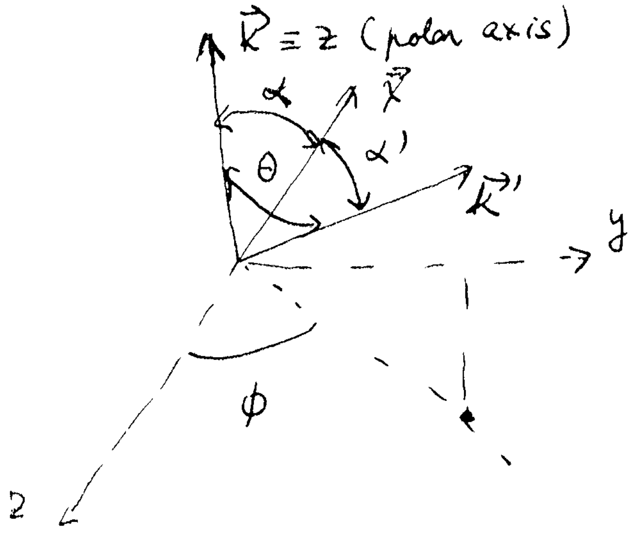
$$f_1(\vec{k}') = \left(\frac{\partial f_0}{\partial \varepsilon'}\right) \vec{\chi}\cdot\vec{k}'$$

For our case of elastic scattering $\varepsilon = \varepsilon'$

$$\Rightarrow \frac{\partial f_0}{\partial \varepsilon} = \frac{\partial f_0}{\partial \varepsilon'}$$

$$\frac{1}{\tau} = \sum_{\vec{k}'} W(\vec{k},\vec{k}')\left(1 - \frac{\vec{\chi}\cdot\vec{k}'}{\vec{\chi}\cdot\vec{k}}\right)$$

To proceed with the calculation we introduce the coordinate system and vectors using spherical coordinates



We define the coordinate system such a way that $\vec{\chi}$ is in yz plane

$$\vec{k} = \begin{pmatrix} 0 \\ 0 \\ k \end{pmatrix} \qquad \vec{\chi} = \begin{pmatrix} 0 \\ \chi \sin\alpha \\ \chi \cos\alpha \end{pmatrix}$$

$$k_x' = k' \sin\theta \cos\phi$$

$$k_y' = k' \sin\theta \sin\phi$$

$$k_z' = k' \cos\theta$$

$$\Rightarrow \quad \vec{\chi}\cdot\vec{k}' = \chi k' \sin\alpha \sin\theta \sin\phi + \chi k' \cos\alpha \cos\theta$$

$$\vec{\chi}\cdot\vec{k} = \chi k \cos\alpha$$

$$\frac{1}{\tau} = \sum_{\vec{k}'} W(\vec{k},\vec{k}')\left(1 - \frac{\chi k \sin\alpha \sin\theta \sin\phi}{\chi k \cos\alpha} + \frac{\chi k \cos\alpha \cos\theta}{\chi k \cos\alpha}\right) =$$

$$= \sum_{\vec{k}'} W(\vec{k},\vec{k}')\left(1 - \operatorname{tg}\alpha \sin\theta \sin\phi + \cos\theta\right)$$

We switch from summation to integration

$$\frac{1}{\tau} = \frac{V}{(2\pi)^3} \int W(\vec{k},\vec{k}')\left(\operatorname{tg}\alpha \sin\theta \sin\phi + \cos\theta - 1\right) d\vec{k}' =$$

$$= \frac{V}{(2\pi)^3} \int_0^{\infty}\int_0^{2\pi}\int_0^{\pi} W(\vec{k},\vec{k}')\left(\operatorname{tg}\alpha \sin\theta \sin\phi + \cos\theta - 1\right) k'^2 dk' \sin\theta \, d\theta \, d\phi$$

Because $\int_0^{2\pi} \sin\phi = 0$ we obtain

$$\frac{1}{\tau} = \frac{V}{(2\pi)^3} \int_0^{\infty}\int_0^{2\pi}\int_0^{\pi} W(\vec{k},\vec{k}') \; (1-\cos\theta) \underbrace{k'^2 \sin\theta \, d\theta \, d\phi \, dk'}_{d\vec{k}'}$$

Returning to summation we have

$$\frac{1}{\tau} = \sum_{\vec{k}'} W(\vec{k},\vec{k}')(1-\cos\theta)$$

Physical meaning of relaxation time

$$\left(\frac{\partial f}{\partial t}\right)_S = -\frac{f_1}{\tau} = -\frac{(f-f_0)}{\tau} \;; \quad \frac{d(f-f_0)}{(f-f_0)} = -\frac{dt}{\tau}$$

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For our case of elastic scattering $\varepsilon = \varepsilon'$

$$\Rightarrow \frac{\partial f_0}{\partial \varepsilon} = \frac{\partial f_0}{\partial \varepsilon'}$$

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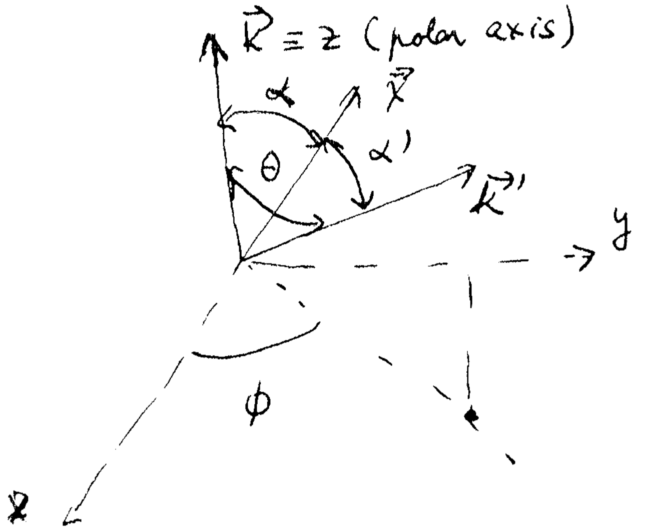

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$$k_x' = k'\sin\theta\cos\phi$$
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$$k_z' = k'\cos\theta$$

$$\Rightarrow \quad \vec{\chi}\cdot\vec{k}' = \chi k'\sin\alpha\sin\theta\sin\phi + \chi k'\cos\alpha\cos\theta$$

$$\vec{\chi}\cdot\vec{k} = \chi k\cos\alpha$$

$$\frac{1}{\tau} = \sum_{\vec{k}'} W(\vec{k},\vec{k}')\left(1 - \frac{\chi k\sin\alpha\sin\theta\sin\phi}{\chi k\cos\alpha} - \frac{\chi k\cos\alpha\cos(\theta)}{\chi k\cos\alpha}\right) =$$

$$= \sum_{\vec{k}'} W(\vec{k},\vec{k}')\left(1 - \operatorname{tg}\alpha\sin\theta\sin\phi - \cos\theta\right)$$

We switch from summation to integration

$$\frac{1}{\tau} = \frac{V}{(2\pi)^3} \int W(\vec{k},\vec{k}')\left(-\operatorname{tg}\alpha \sin\theta \sin\phi - \cos\theta + 1\right) d\vec{k}' =$$

$$= \frac{V}{(2\pi)^3} \int_0^{\infty}\int_0^{2\pi}\int_0^{\pi} W(\vec{k},\vec{k}')\left(-\operatorname{tg}\alpha \sin\theta \sin\phi - \cos\theta + 1\right) k'^2 dk' \sin\theta\, d\theta\, d\phi$$

Because $\int_0^{2\pi} \sin\phi = 0$ we obtain

$$\frac{1}{\tau} = \frac{V}{(2\pi)^3} \int_0^{\infty}\int_0^{2\pi}\int_0^{\pi} W(\vec{k},\vec{k}')\ (1-\cos\theta)\, \underbrace{k'^2 \sin\theta\, d\theta\, d\phi\, dk'}_{d\vec{k}'}$$

Returning to summation we have

$$\frac{1}{\tau} = \sum_{\vec{k}'} W(\vec{k},\vec{k}')(1-\cos\theta)$$

Calculation of relaxation time

During scattering of carriers several scattering mechanisms can be simultaneously active. The resulting relaxation time can be calculated using the so called Matthiessen rule

$$\frac{1}{\tau} = \sum_i \sum_{\vec{k}'} W_i(\vec{k},\vec{k}')(1-\cos\theta_i) = \sum_i \frac{1}{\tau_i}$$

Here i is an index of the scattering mechanism. The Matthiessen rule can be derived from the probability theory - the scattering mechanisms are alternative, therefore the probabilities W_i are summed (the probability rule of summing of probabilities.)

When calculating τ_i we switch from summation to integration, it means that we have to multiply the integral with the density of states in the k' space

$$g_{3D}(k') = \frac{V}{(2\pi)^3} = \frac{L^3}{(2\pi)^3}$$

Here V is the volume of the sample with a shape of cube with side L

$$\frac{1}{\tau_i} = \underbrace{\frac{V}{(2\pi)^3}}_{g_{3D}(k')} \int_{\vec{k}'} W_i(\vec{k},\vec{k}')(1-\cos\theta_i)\,d\vec{k}' =$$

$$= \underbrace{\int_0^{2\pi} d\varphi}_{2\pi} \int_0^{\pi} \underbrace{\int_0^{\infty} \frac{V}{(2\pi)^3} W_i(\vec{k},\vec{k}')\, k'^2 dk'}_{W_i(k,\theta_i)} (1-\cos\theta_i)\, d\theta_i =$$

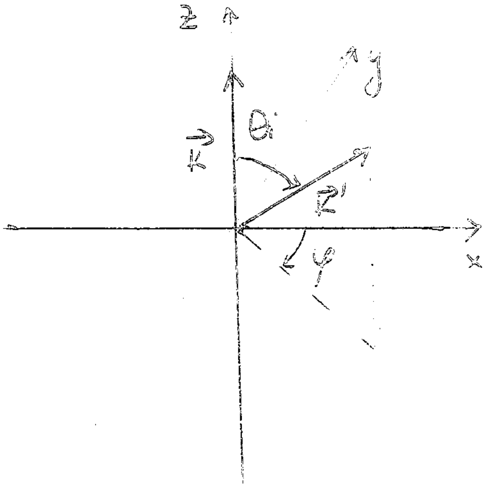
$$= 2\pi \int_0^{\pi} W_i(k,\theta_i)(1-\cos\theta_i)\, d\theta_i$$

We switched to spherical coordinates k', θ_i, φ

$$d\vec{k}' = k'^2 \sin\theta_i \, d\theta_i \, d\varphi \, dk'$$

We have chosen the polar axis ∥ to $\vec{k}'$

θ_i is representing both the scattering angle and polar angle in this case.



We also introduced

$$W_i(k,\theta_i) = \frac{V}{(2\pi)^3} \int_0^{\infty} k'^2 W_i(\vec{k},\vec{k}')\, dk'$$

To proceed with the calculation we have to use some formula for $W_i(\vec{k},\vec{k}')$

We use the Fermi golden rule

$$W_i(\vec{k},\vec{k}') = \frac{2\pi}{\hbar} |M_i(\vec{k},\vec{k}')|^2 \delta(\varepsilon(\vec{k})-\varepsilon(\vec{k}'))$$

$M_i(\vec{k},\vec{k}')$ .. Matrix element of transition from state $\vec{k}$ to $\vec{k}'$

$\delta(\varepsilon(\vec{k})-\varepsilon(\vec{k}'))$ Law of energy conservation for elastic scattering

$$M_i(\vec{k},\vec{k}') = \frac{1}{V}\int \Psi^*_{\vec{k}'}(\vec{r}) H' \Psi_{\vec{k}}(\vec{r})\, d\vec{r}$$

Ψ .. wave function of electron and scattering center

H' .. interaction Hamiltonian

$$W_i(k,\theta_i) = \frac{V}{(2\pi)^3}\frac{2\pi}{\hbar}\int_0^\infty |M_i(\vec{k},\vec{k}')|^2 \delta(\varepsilon(\vec{k})-\varepsilon(\vec{k}'))\, k'^2\, dk'$$

Let us introduce $\varepsilon(\vec{k}) = \varepsilon$ $\quad \varepsilon(\vec{k}') = \varepsilon'$

$$\varepsilon' = \frac{\hbar^2 k'^2}{2m_c^*} \rightarrow k' = \frac{\sqrt{2m_c^*\varepsilon'}}{\hbar}$$

$$dk' = \frac{\sqrt{2m_c^*}}{2\sqrt{\varepsilon'}\,\hbar}\, d\varepsilon'$$

$$W_i(k,\theta_i) = \frac{V}{4\pi^2\hbar}\int_0^\infty |M_i(\vec{k},\vec{k}')|^2 \delta(\varepsilon-\varepsilon')\, \frac{2m_c^*\varepsilon'}{\hbar^2}\cdot\frac{\sqrt{2m_c^*}}{2\sqrt{\varepsilon'}\,\hbar}\, d\varepsilon'$$

$$W_i(k,\theta_i) = \frac{V}{4\hbar}\int_0^\infty |M_i(\vec{k},\vec{k}')|^2 g_{3D}(\varepsilon')\,\delta(\varepsilon-\varepsilon')\,d\varepsilon'$$

We have used the formula for density of states in the energy space in 3D

$$g_{3D}(\varepsilon') = \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{\varepsilon'}$$

$$\Rightarrow \quad W_i(k,\theta_i) = \frac{V}{4\hbar}|M_i(\vec{k},\vec{k}')|^2 g(\varepsilon)$$

We assumed that $M_i(\vec{k},\vec{k}')$ does not depend on energy and used the properties of δ- function

Now we proceed with calculation of τ_i

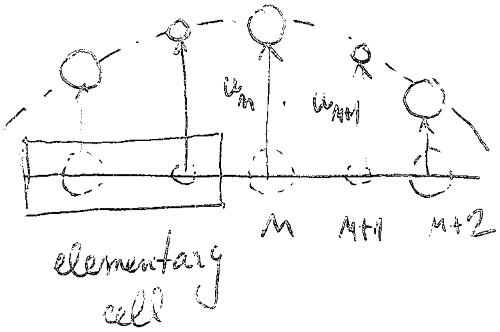
$$\frac{1}{\tau_i} = 2\pi g(\varepsilon)\int_0^\pi \frac{V}{4\hbar}|M_i(\vec{k},\vec{k}')|^2(1-\cos\theta_i)\sin\theta_i\,d\theta_i$$

To evaluate τ_i one has to know the matrix element for each scattering mechanism

We will now continue to discuss individual scattering mechanisms

Scattering on acoustic phonons (non-polar)

From the theory we know that in case of acoustic vibrations (acoustic phonons) atoms in the elementary cell vibrate in phase.



Example - elementary cell with 2 atoms (GaAs, InSb, CdTe) or even Si (elementary semiconductor but 2 Si atoms in the elementary cell are different due to different bond strengths)

$\vec{u}_n$ ... displacement of the n-th atom

$\vec{u}_{n+1}$ ... displacement of the (n+1)th atom etc

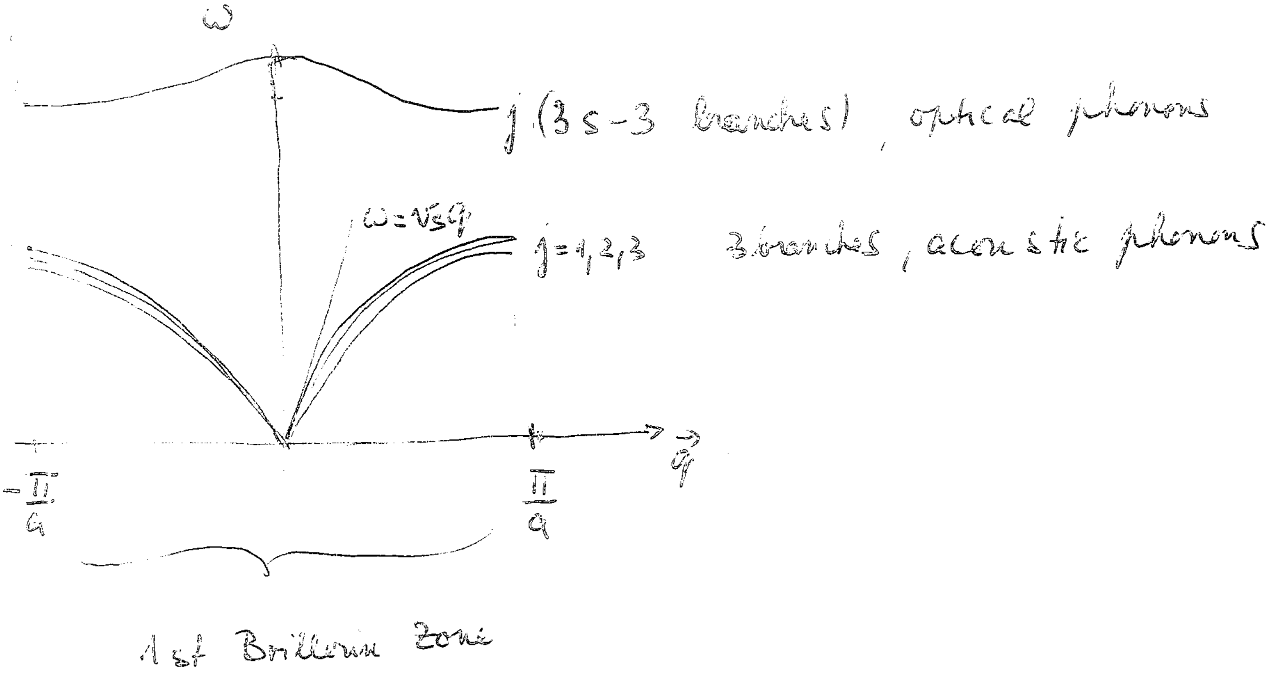
In the acoustic vibration the displacements of the neighbor atoms are similar - in the same direction („are in phase")

$$\vec{u}_{n,l} = \frac{1}{\sqrt{N}} \sum_{\vec{q},j} \left\{ \vec{e}_{lj}(\vec{q}) b_j(\vec{q}) e^{i\vec{q}\vec{a}_n} + \vec{e}^{\,*}_{l,j}(\vec{q}) b_j^*(\vec{q}) e^{-i\vec{q}\vec{a}_n} \right\}$$

$\vec{e}_{l,j}$. vector of polarization - determines the direction of oscillation of the l-th atom participating in a monochromatic lattice wave with wave vector $\vec{q}$. j .. is the index of the phonon branch with frequency $\omega_j(\vec{q})$

The scattering of carriers on acoustic phonons takes place because due to propagation of elastic wave the elementary cell is deformed. This results in the change of the lattice constant. In case of long waves $(q \to 0)$ the interaction Hamiltonian can be written as

$$H'_{LA} = E_1 \operatorname{div} \vec{u}_{LA}(\vec{r}) \rightarrow H'_{LA} \sim i\vec{q}\cdot\vec{e}_{\vec{q},j}$$



Because $H'_{LA} \sim i\vec{q}\cdot\vec{e}_{\vec{q},j}$, $H'_{LA} = 0$ if $\vec{q} \perp \vec{e}_{\vec{q},j}$

$\vec{q}$ .. direction of wave propagation

$\vec{e}_{\vec{q},j}$ .. direction of oscillation of atoms in the wave

It means, that only longitudinal phonons $(\vec{q} \parallel \vec{e}_{\vec{q},j})$

participate in the interaction ($H'_{LA} \neq 0$)

Now we will show that only long-wave phonons participate in the interaction with free carriers

The scattering on phonons is in general non-elastic. We will, however, use the relaxation time approximation for situations, when the change of energy of carrier at scattering is small.

To show, that only long-wave phonons participate in interactions, we will calculate the conservation of momentum and energy during the interaction.

$$\vec{k}' = \vec{k} \pm \vec{q}$$

$$\vec{k}'^2 = \vec{k}^2 \pm 2\vec{k}\vec{q} + \vec{q}^2 = k^2 + 2kq\cos\theta + q^2$$

$\varepsilon(\vec{k}') = \varepsilon(\vec{k}) \pm \hbar\omega_{\vec{q}}$ $\omega_{\vec{q}}$ frequency of acoustic phonon

$$\frac{\hbar^2 k'^2}{2m_e^*} = \frac{\hbar^2 k^2}{2m_e^*} \pm \hbar\omega_q$$

$$\frac{\hbar^2 k^2}{2m_e^*} \pm \frac{\hbar^2}{2m_e^*}2kq\cos\theta + \frac{\hbar^2 q^2}{2m_e^*} = \frac{\hbar^2 k^2}{2m_e^*} \pm \hbar\omega_q$$

$$q^2 = \mp 2kq\cos\theta \pm \frac{2m_e^*}{\hbar}\omega_q$$

$$q = 2k\{\mp\cos\theta \pm \frac{m_e^*}{\hbar k q}\omega_q)$$

$$m_e^* v = \hbar k$$

$$q = 2k\left(\mp\cos\theta \pm \frac{\omega_q}{v q}\right) \qquad \omega_q = \underset{\uparrow}{v_s}\cdot q$$

velocity of acoustic wave

$$q = 2k\left(\mp\cos\theta \pm \frac{v_s}{v}\right)$$

$$q_{max} = 2k\left(1 + \frac{v_s}{v}\right) \qquad \begin{array}{l} v_s \sim 10^5\ m/s \\ v \approx 10^7\ m/s \end{array}$$

$$\Rightarrow \quad q_{max} \approx 2k$$

$$\frac{q_{max}}{\frac{\pi}{a}} \approx \frac{2 m_e^* v}{\hbar \cdot \frac{\pi}{a}} \approx 1/4$$

$\Rightarrow$ only acoustic waves with wave vector from the interval between 0 and $\frac{\pi}{4a}$ ($1/4$ of the Brillouin zone)

participate in the interaction with electrons (or holes)

The matrix element for scattering on non-polar optical phonons (longitudinal) holds

$$|M_{LA}(\vec{k},\vec{k}')|^2 = E_{1,c}^2\, k_B T\, \frac{1}{\rho\, v_s^2\, V}$$

E_{1c} … deformation potential of the conduction band (material parameter)

ρ … density of the matter

The relaxation time for scattering on long-wave non-polar longitudinal acoustic phonons is

$$\frac{1}{\tau_{LA}} = \frac{\pi V}{2\hbar} g(\varepsilon) \int_0^{\pi} |M_{LA}|^2 (1-\cos\theta)\sin\theta \, d\theta$$

$$\frac{1}{\tau_{LA}} = \frac{\pi V}{2\hbar} \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3} \varepsilon^{1/2} \frac{E_{ac}^2 k_B T}{\rho v_s^2 V} \underbrace{\int_0^{\pi} (1-\cos\theta)\sin\theta \, d\theta}_{-\int_1^{-1}(1-x)\,dx = 2}$$

$$\Rightarrow \quad \frac{1}{\tau_{LA}} \sim \varepsilon^{1/2} \; k_B T \qquad \varepsilon \sim k_B T$$

$$\Rightarrow \quad \frac{1}{\tau_{LA}} \sim (k_B T)^{3/2} \qquad \tau_{LA} \sim (k_B T)^{-3/2}$$

$$\log \tau_{LA} \sim -3/2 \log T$$

Scattering on polar acoustic phonons

In crystals without a center of symmetry with a partial ionic bond there is present also perturbation Hamiltonian connected with electric dipole of the oscillation

The resulting relaxation time $\tau_{AP}^{(P)}$ is

$$\tau_{AP}^{(P)} = \tau_{PZ} \sim T^{-1/2}$$

The scattering on polar acoustic phonons is also called piezoelectric scattering, because piezoelectric effect is present in these types of crystals.

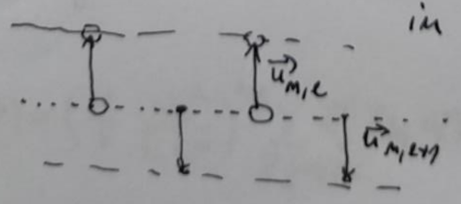
Scattering on non-polar optical phonons

The atoms of the elementary cell oscillate in anti-phase

The interaction Hamiltonian is

$$H'^{(NP)}_{LO} = \frac{\pi}{a} \cdot D_0 \cdot \vec{u}$$

u .. shift of atoms in the long wave



$$\vec{u} = \vec{u}_{M,l} - \vec{u}_{M,l+1}$$

Scattering on polar optical phonons

The atoms of the base vibrate in anti-phase. Due to presence of electric charges vibrations cause a time dependent electric dipole.

We will suppose a base of two atoms

$$\vec{u}_{n,l}(\vec{q}) = \frac{1}{\sqrt{N}} \left\{ \vec{e}_{l,j}(\vec{q}) b_j(\vec{q}) e^{i\vec{q}\cdot\vec{a}_n} + c.c. \right\}$$

$\vec{u}_{n,l}(\vec{q})$ is the displacement of the n-th atom of the j-th branch with wave vector $\vec{q}$,

l in the index of atom in the elementary cell ($l = 1,2$ in our case)

$\vec{e}$ is the polarization vector

$\vec{a}_n$ ... lattice vector of the n-th cell

Long-wavelength vibrations in optical branch of a crystal with ionic or partially ionic bond result in polarization of the lattice

We know from the results of solid state theory, that $\vec{P}$ in this case can be written as

$$\vec{P}(\vec{r}) = \left(\frac{M}{V} \cdot \frac{\omega_0^2}{\varepsilon_0 \varepsilon_r^*}\right)^{1/2} \sum_{\vec{q}, j=4,5,6} \vec{e}_j \left(b_j(\vec{q}) e^{i\vec{q}\cdot\vec{r}} + b_j^*(q) e^{-i\vec{q}\cdot\vec{r}}\right)$$

Where $M = M_1 + M_2$, ω_0 is the average frequency of optical phonons, $\vec{e}_j$ is a unit vector related to polarization vectors of two atoms in the elementary cell by relations

$$\vec{e}_{1j} = \left(\frac{M_2}{M_1}\right)^{1/2} \vec{e}_j \qquad \vec{e}_{2,j} = -\left(\frac{M_1}{M_2}\right)^{1/2} \vec{e}_j .$$

$$\vec{P} = \vec{D} - \varepsilon_0 \vec{E} \quad \Rightarrow \quad \mathrm{div}\, \vec{E} = \frac{1}{\varepsilon_0}\left(\mathrm{div}\, \vec{D} \underbrace{- \mathrm{div}\, \vec{P}}_{\rho'}\right) =$$

$$= \frac{1}{\varepsilon_0}(\rho + \rho')$$

ρ ... density of free charge

ρ' .. equivalent density of charge describing the influence of the dielectrics on electric field

We will assume that the density of free charge $\rho = 0$. Then

$$\mathrm{div}\, \vec{E} = \frac{\rho'}{\varepsilon_0} \qquad \vec{E} = -\nabla_r \varphi \qquad \Delta\varphi = -\frac{\rho'}{\varepsilon_0}$$

Poisson equation

$$\Rightarrow \Delta\varphi = \frac{\mathrm{div}\, \vec{P}}{\varepsilon_0}$$

In our case

$$\mathrm{div}\, \vec{P}(\vec{r}) = \left(\frac{M}{V}\frac{\omega_0^2}{\varepsilon_0 \varepsilon_r}\right)^{1/2} \sum_{\vec{q},j} i \underbrace{(\vec{q} \cdot \vec{e}_{qj}(\vec{q})}_{\neq 0 \text{ only if } \vec{q} \parallel \vec{e}_{qj}} \{ b_j(\vec{q}) e^{i\vec{q}\cdot\vec{r}} + \text{c.c.} \}$$

If $\Delta\varphi(\vec{r}) \sim (\vec{q}\cdot\vec{e}_{q,j}(\vec{q}))$ then also

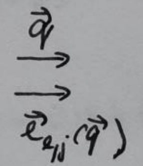
$\nabla_{\vec{r}}\varphi$ and $\varphi \sim \vec{q}\cdot\vec{e}_{q,j}(\vec{q})$

(the term $\vec{q}\cdot\vec{e}_{q,j}(\vec{q})$ does not depend on $\vec{r}$, so remains unchanged when integrating $\Delta\varphi(\vec{r})$ and $\nabla_{\vec{r}}\varphi(\vec{r})$ over $\vec{r}$

⇒ the interaction Hamiltonian

$$H' = -e\varphi \sim \vec{q}\cdot\vec{e}_{q,j}(\vec{q})$$

⇒ The scattering happens only on longitudinal optical phonons



The scattering on optical phonons is in general non-elastic. It means that the relaxation time approximation can be used only in the case that nonelasticity is small. This happens at high temperatures $T \gg \frac{\hbar\omega_0}{k_B}$

In this case the energy of electron is high compared to the energy of electron.

In this case $|\vec{q}| \ll |\vec{k}|$; $\vec{k}' = \vec{k} \pm \vec{q} \approx \vec{k}$

We will use the matrix element

↓ absorption of phonon

$$|M_{LO}|^2 = \sum_{+,-} \frac{e^2\hbar\omega_{LO}}{2V\varepsilon_0}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_s}\right)\cdot\frac{1}{k^2}\,F_q \begin{Bmatrix} n_q \\ n_q+1 \end{Bmatrix}$$

↗ emission of phonon

$$n_q = \frac{1}{e^{\frac{\hbar\omega_{LO}}{k_BT}}-1} \qquad F_q = \frac{k^2}{\frac{1}{R_s^2}+q^2}$$

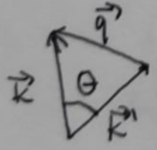
R_s … screening length

If we neglect screening ($R_S\to\infty$; $F_q \sim \frac{k^2}{q^2}$)

$$\frac{1}{\tau_{LO}^{(+)}} = \sum_{+,-}\frac{\pi V}{2\hbar}\,\frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3}\cdot\sqrt{E}\int_0^{\pi}\frac{e^2\hbar\omega_{LO}}{2V\varepsilon_0}\cdot\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_s}\right)\cdot\frac{1}{q^2}\begin{Bmatrix} n_q \\ n_q+1 \end{Bmatrix}\cdot$$

$$\cdot\,(1-\cos\theta)\sin\theta\, d\theta$$

$\vec{q} = \vec{k}-\vec{k}'$; if $|\vec{k}|\approx|\vec{k}'|$ .. elastic scattering, then



$$|\vec{q}| = 2|\vec{k}|\sin\frac{\theta}{2} \Rightarrow q^2 = 2k^2(1-\cos\theta)$$

$|\vec{k}| \equiv k$

$|\vec{q}| \equiv q$

$$\frac{1}{q^2} = \frac{1}{2k^2(1-\cos\theta)} = \frac{\hbar^2}{4m_e^* E}\cdot\frac{1}{1-\cos\theta}$$

$$\frac{1}{\tau_{LO}^{(P)}} = \sum_{+,-} C\,\varepsilon^{1/2} \int_0^{\pi} \frac{1}{q^2} \cdot \left\{ \begin{matrix} n_q \\ n_q+1 \end{matrix} \right\} (1-\cos\theta)\sin\theta\, d\theta$$

$$C = \frac{\pi V}{2\hbar} \frac{(2m_e^*)^{3/2}}{2\pi^2 \hbar^3} \frac{e^2 \hbar\omega_{LO}}{2V\varepsilon_0} \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s} \right)$$

$$\frac{1}{\tau_{LO}^{(P)}} = \sum_{+,-} C\,\varepsilon^{1/2} \frac{\hbar^2}{4m_e^*\varepsilon} \int_0^{\pi} \frac{(1-\cos\theta)}{(1-\cos\theta)} \sin\theta\, d\theta \left\{ \begin{matrix} n_q \\ n_q+1 \end{matrix} \right\} =$$

$$= C \frac{\hbar^2}{4m_e^*} \varepsilon^{-1/2} \int_0^{\pi} (\underbrace{n_q + n_q + 1}_{\approx 2n_q}) \cdot \sin\theta\, d\theta$$

$$n_q = \frac{1}{e^{\frac{\hbar\omega_{LO}}{k_BT}} - 1}$$; at high temperatures $\frac{\hbar\omega_{LO}}{k_BT}$ is small

$$\Rightarrow e^{\frac{\hbar\omega_{LO}}{k_BT}} \approx 1 + \frac{\hbar\omega_{LO}}{k_BT}$$

$$\Rightarrow n_q \approx \frac{k_BT}{\hbar\omega_{LO}} \qquad \int_0^{\pi} \sin\theta\, d\theta = 2$$

$$\frac{1}{\tau_{LO}^{(P)}} = C \cdot \frac{\hbar^2}{4m_e^*} \varepsilon^{-1/2} \cdot \frac{4k_BT}{\hbar\omega_{LO}} \qquad \varepsilon \propto k_BT$$

$$\Rightarrow \frac{1}{\tau_{LO}^{(P)}} \approx T^{1/2} \quad ; \quad \tau_{LO}^{(P)} \approx T^{-1/2}$$

$$\log \tau_{LO}^{(P)} \approx -1/2 \log T$$

Summary of scattering for phonons at a high-temperature limit (when this type of scattering usually dominates)

Non-polar acoustic phonons	$\tau_{LA} \sim T^{-3/2}$
Polar acoustic phonons	$\tau_{PZ} \sim T^{-1/2}$
Non-polar optical phonons	$\tau_{LO}^{(np)} \sim T^{-3/2}$
Polar optical phonons	$\tau_{LO}^{(p)} \sim T^{-1/2}$

Scattering on ionized impurities

$$\frac{1}{\tau_I} \sim \varepsilon^{-3/2} \quad (\sim T^{-3/2})$$

$$\tau_I \sim T^{3/2}$$

Combined scattering on ionized impurities and phonons (presented for acoustic phonons)

$$\frac{1}{\tau} = \frac{1}{\tau_I} + \frac{1}{\tau_{LA}}$$

We will continue with description of scattering on ionized impurities.

As an example let us calculate $M_i(\vec{k},\vec{k}')$ for scattering on ionized impurities

The perturbing potential is the so-called "screened Coulomb potential"

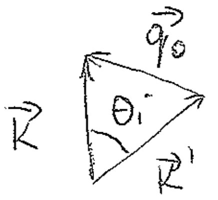
$$\varphi = \pm \frac{e}{4\pi\varepsilon_0\varepsilon_r r}\cdot e^{-\frac{r}{R_S}}$$

Here R_S is the so called screening length

The screening happens due to mobile carriers (electrons or holes) that are attracted to impurity atoms by Coulomb force and effectively decrease the Coulomb force between the screened impurity atom and test charge.

The corresponding interaction Hamiltonian is then

$$H' = \pm e\varphi$$



Let us define $\vec{q} = \vec{k} - \vec{k}'$

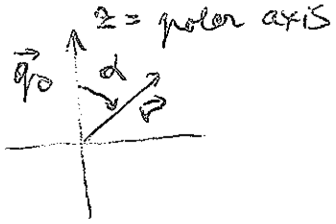
$$q_0 = 2k\sin\frac{\theta_i}{2}$$

$|\vec{k}| = |\vec{k}'|$

~ elastic scattering

We will now calculate $M_I(\vec{k},\vec{k}')$ using polar coordinates r, α, φ

We will align the polar axis with vector $\vec{q}_0$



We will choose a plane wave as $\Psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}}$

$$M_i(\vec{k},\vec{k}') = \frac{1}{V}\,\frac{e^2}{4\pi\varepsilon_0\varepsilon_r}\int_0^{2\pi} d\varphi \int_0^{\pi}\int_0^{\infty}\frac{1}{r}\,e^{-\frac{r}{R_s}}\,e^{i\overbrace{(\vec{k}-\vec{k}')}^{\vec{q}_0}\vec{r}}\,r^2 dr \sin\alpha\, d\alpha =$$

$$= \frac{e^2}{2\varepsilon_0\varepsilon_r V}\int_0^{\infty} r e^{-\frac{r}{R_s}}\int_0^{\pi} e^{iq_0 r\cos\alpha}\sin\alpha\, d\alpha\, dr =$$

$$\cos\alpha = t \qquad -\sin\alpha\, d\alpha = dt$$

$$= \frac{e^2}{2\varepsilon_0\varepsilon_r V}\int_0^{\infty} r e^{-\frac{r}{R_s}}\int_{+1}^{-1} -e^{iq_0 r t}\, dt\, dr =$$

$$= \frac{e^2}{2\varepsilon_0\varepsilon_r V}\int_0^{\infty} r e^{-\frac{r}{R_s}}\left[\frac{e^{iq_0 r t}}{iq_0 r}\right]_{-1}^{+1} dr =$$

$$= \frac{e^2}{2\varepsilon_0\varepsilon_r V}\int_0^{\infty} r e^{-\frac{r}{R_s}}\,\frac{2i\sin q_0 r}{iq_0 r}\, dr =$$

$$= \frac{e^2}{2\varepsilon_0\varepsilon_r q}\int_0^{\infty}\underbrace{e^{-\frac{r}{R_s}}\,e^{iq_0 r}\, dr}_{\text{table integral}}$$

$$\int e^{ar}\sin br\, dr = \frac{e^{ar}}{a^2+b^2}\left(a\sin br - b\cos br\right)$$

We set $q = -\frac{1}{R_S}$ $b = q_0$

$$M_i(\vec{k},\vec{k}') = \frac{e^2}{V\varepsilon_0\varepsilon_r q_0}\left[\frac{1}{\left(\frac{1}{R_S}\right)^2 + q_0^2}\left(-\frac{e^{-\frac{r}{R_S}}}{R_S}\sin q_0 r - e^{-r/R_S}\cos q_0 r\right)\right]_0^\infty =$$

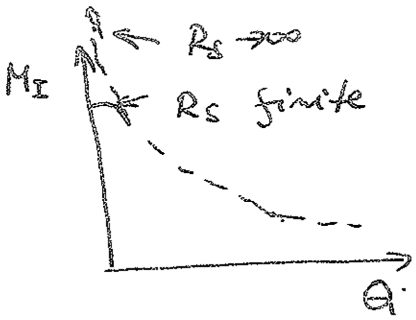
$$= \frac{e^2}{V\varepsilon_0\varepsilon_r q_0}\left(\frac{1}{\left(\frac{1}{R_S}\right)^2 + q_0^2}\right) q_0 = \frac{e^2}{V\varepsilon_0\varepsilon_r}\cdot\frac{1}{\left(\frac{1}{R_S^2}\right)^2 + q_0^2}$$

$q_0 = 2k\sin\frac{\theta_i}{2}$

$\theta_i \to 0$ $q_0 \to 0$

for $R_S \to \infty$ $M_I \to \infty$

(unscreened)



$N_I = \frac{N}{V}$

concentration of impurities

$$\frac{1}{\tau_I} = \frac{\pi V}{2\hbar} g(\varepsilon) N_I \int_0^\pi |M_I|^2 (1-\cos\theta_i)\sin\theta_i \, d\theta_i$$

$$\frac{1}{\tau_I} = \frac{\pi V}{2\hbar} g(\varepsilon) N_I \int_0^\pi \left(\frac{e^2}{V\varepsilon_0\varepsilon_r}\right)^2 \cdot \left(\frac{1}{\frac{1}{R_S^2} + q_0^2}\right)^2 (1-\cos\theta_i)\sin\theta_i \, d\theta_i$$

$q_0^2 = 4k^2\sin^2\frac{\theta_i}{2} = 2k^2(1-\cos\theta_i)$ $\varepsilon = \frac{\hbar^2 k^2}{2m_e^*}$ $k^2 = \frac{2m_e^*\varepsilon}{\hbar^2}$

$$\frac{1}{\tau_I} = \frac{\pi V}{2\hbar} g(\varepsilon)\left(\frac{e^2}{V\varepsilon_0\varepsilon_r}\right)^2 \cdot N_I \int_0^\pi \frac{(1-\cos\theta_i)\sin\theta_i \, d\theta_i}{\left(\frac{4m_e^*\varepsilon}{\hbar^2}(1-\cos\theta_i) + \frac{1}{R_S^2}\right)^2} =$$

$$= \frac{\pi V}{2\hbar} g(\varepsilon)\left(\frac{e^2}{V\varepsilon_0\varepsilon_r}\right)^2 \cdot \left(\frac{\hbar^2}{4m_e^*\varepsilon}\right)^2 N_I \int_0^\pi \frac{(1-\cos\theta_i)\sin\theta_i \cdot d\theta_i}{\left(1-\cos\theta_i + \frac{\hbar^2}{4m_e^*\varepsilon R_S^2}\right)^2} =$$

$$= \frac{\pi V}{2\hbar} g(\varepsilon) \left(\frac{e^2}{V\varepsilon_0\varepsilon_r}\right)^2 \cdot \left(\frac{\hbar^2}{4m_e^*\varepsilon}\right)^2 N_I \int_0^2 \frac{t\,dt}{(t+b)^2} =$$

(substitution $1-\cos\theta = t$)

$$= \frac{\pi V}{2\hbar} g(\varepsilon) \left(\frac{e^2}{V\varepsilon_0\varepsilon_r}\right)^2 \left(\frac{\hbar^2}{4m_e^*\varepsilon}\right)^2 N_I \left[\underbrace{\left(\frac{-2}{b+2}\right) + \ln\left(\frac{b+2}{2}\right)}_{\text{This term is only weakly dependent on energy}} \right]$$

$$\Rightarrow \frac{1}{\tau_I} \sim \varepsilon^{1/2} \cdot \frac{1}{\varepsilon^2} \sim \varepsilon^{-3/2}$$

$$\Rightarrow \tau_I \sim \varepsilon^{3/2} \quad (T^{3/2})$$

We have used the integral

$$\int \frac{t}{T^2}\,dt = \frac{b}{a^2 T} + \frac{1}{a^2} \ln T$$

$$T = at + b$$

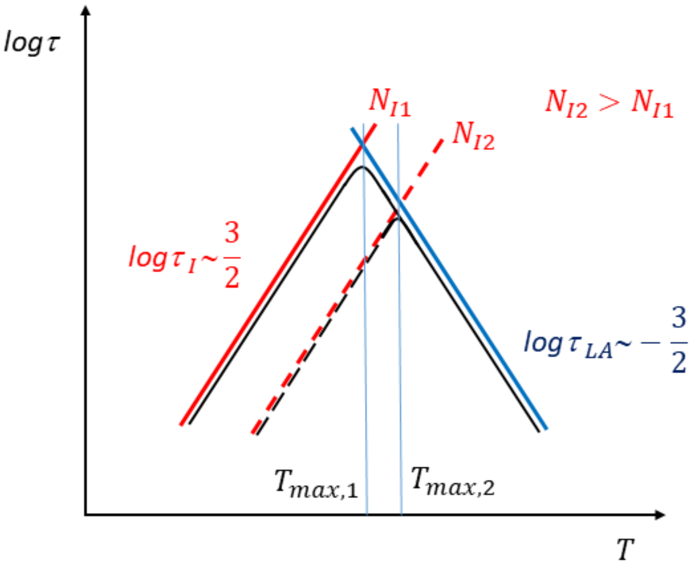
in our case $a = 1$

$$\int \frac{t}{(b+t)^2}\,dt = \frac{b}{b+t} + \ln(b+t)$$

$$\left[\frac{b}{b+t} + \ln(b+t)\right]_0^2 = \frac{b}{2+b} - 1 + \ln\left(\frac{b+2}{b}\right) =$$

$$= \frac{-2}{b+2} + \ln\left(\frac{b+2}{b}\right)$$

The following picture shows an example of application of the Matthiessen rule for a combination of two scattering mechanisms – scattering on ionized impurities and non-polar acoustical phonons.



We can see that the relaxation time has a maximum for a given concentration of ionized impurities. If this concentration is higher, the maximum is smaller and is shifted gto higher temperature. Multiplying the „y“ axis by $\frac{e}{m^*}$ we obtain the diagram for the temperature dependence of mobility $\mu = \frac{e}{m^*}\tau$.

Solution of Boltzmann transport equation

$$\frac{\partial f}{\partial t} = -\vec{v}\nabla_{\vec{r}} f - \vec{a}\nabla_{\vec{v}} f - \frac{f_1}{\tau} \qquad f = f_0 + f_1$$

$$m_e^* v = \hbar k \qquad \nabla_{\vec{v}} = \frac{m_e^*}{\hbar}\nabla_{\vec{k}}$$

$$m_e^* dv = h\, dk \quad \nearrow$$

$$\Rightarrow \frac{d}{dv} = \frac{m_e^*}{\hbar}\frac{d}{dk}$$

$$\Rightarrow \frac{\partial f}{\partial t} = -\vec{v}\cdot\nabla_{\vec{r}} f - \frac{\vec{F}}{m_e^*}\cdot\frac{m_e^*}{\hbar}\nabla_{\vec{k}} f - \frac{f_1}{\tau}$$

Let us show an example of a solution for a simple situation – application of $\vec{E}$-field in a homogeneous semiconductor in a stationary case (i.e. $\frac{\partial f}{\partial t} = 0$)

Homogeneous semiconductor ≡ $\nabla_{\vec{r}} f = 0$

$\vec{E}$-field → $\vec{F} = -eEx$

$$F_x = -eE_x$$

⇒ BTE reduces to $\frac{1}{\hbar}\vec{F}\cdot\nabla_{\vec{k}} f = -\frac{f_1}{\tau}$

$$x: \quad -\frac{e}{\hbar}E_x\frac{\partial f}{\partial k_x} = -\frac{f_1}{\tau}$$

$$\Rightarrow \quad f_1 = -\frac{\tau}{\hbar}F_x\frac{\partial f}{\partial k_x} = \frac{\tau}{\hbar}eE_x\cdot\frac{\partial f}{\partial k_x}$$

$$\frac{\partial f}{\partial k_x} = \frac{\partial f}{\partial \mathcal{E}}\cdot\frac{\partial \mathcal{E}}{\partial k_x} \quad ; \quad \frac{\partial \mathcal{E}}{\partial k_x} = \frac{\hbar^2 k_x}{m_e^*} = \hbar v_x$$

$$(m_e^* v_x = \hbar k_x)$$

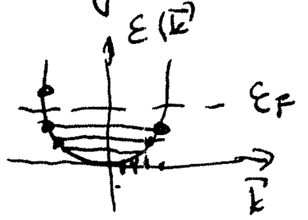
$$\Rightarrow f_1 = -\tau v_x F_x\cdot\frac{\partial f_0}{\partial \mathcal{E}} = \tau v_x e E_x\frac{\partial f_0}{\partial \mathcal{E}}$$

Electric current

We have shown previously that

$$j = \rho_c v \qquad \rho_c \ldots \text{density of electric charge}$$

$$\rho_c = \frac{-2e}{V}\sum_{\vec k} f(\vec k)$$



$$j = -\frac{2e}{V}\sum_{\vec k} f(\vec k)\,\vec v(\vec k)$$

We switch from summation to integration multiplying by density of states in k space $\frac{V}{(2\pi)^3}$

$$\vec j_x = -\frac{2e}{V}\cdot\frac{V}{8\pi^3}\int f(\vec k)\,\vec v(\vec k)\,d^3\vec k \qquad j_x = -\frac{2e}{V}\cdot\frac{V}{8\pi^3}\int f(\vec k)\,v_x\,d^3\vec k$$

$$f(\vec k) = f_0(\vec k) - \tau v_x(-eE_x)\frac{\partial f}{\partial \varepsilon}$$

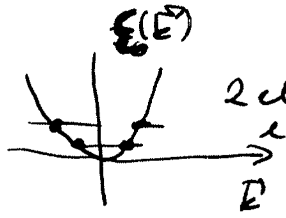
$$j_x = -\frac{e}{4\pi^3}\int v_x f_0(\vec k)\,d^3\vec k - \frac{e^2}{4\pi^3}E_x\int \tau v_x^2\frac{\partial f_0}{\partial \varepsilon}\,d^3\vec k$$

Since ε is an even function of $\vec k$, $v_x f_0(\vec k)$ is an odd function v_x. Since integration with respect to dk_x ranges from $(-\infty$ to $+\infty)$ the first term on the right hand side becomes zero and only the second term remains

$$j_x = -\frac{e^2 E_x}{4\pi^3}\int \tau v_x^2\frac{\partial f_0}{\partial \varepsilon}\,d^3\vec k$$

We can express the electron density n as

$$n = 2 \cdot \frac{\sum_{\vec{k}} f(\vec{k})}{V} =$$



2 electrons in each state

$$= \frac{2}{V} \cdot \underbrace{\frac{V}{(2\pi)^3}}_{} \cdot \int f(\vec{k})\, d^3\vec{k} = \frac{1}{4\pi^3} \int f_0(\vec{k})\, d^3\vec{k}$$

$g_{\vec{k}}$ .. density of states in $\vec{k}$-space

We can then write

$$j_x = -\frac{e^2 n E_x}{\cancel{4\pi^3}} \cdot \cancel{4\pi^3} \frac{\int \tau v_x^2 \frac{\partial f_0}{\partial \varepsilon}\, d^3\vec{k}}{\int f_0\, d^3\vec{k}} =$$

$$= -e^2 n E_x \frac{\int \tau v_x^2 \frac{\partial f_0}{\partial \varepsilon}\, d^3\vec{k}}{\int f_0\, d^3\vec{k}}$$

$$\frac{\partial f_0}{\partial \varepsilon} = -\frac{1}{k_B T} \cdot \frac{e^{\frac{\varepsilon - \varepsilon_F}{k_B T}}}{\left(1 + e^{\frac{\varepsilon - \varepsilon_F}{k_B T}}\right)^2} = -\frac{1}{k_B T} f_0 (1 - f_0)$$

because $1 - f_0 = 1 - \frac{1}{1 + e^{\frac{\varepsilon - \varepsilon_F}{k_B T}}} = \frac{e^{\frac{\varepsilon - \varepsilon_F}{k_B T}}}{1 + e^{\frac{\varepsilon - \varepsilon_F}{k_B T}}}$

We introduce $\phi(\varepsilon) = \tau f_0 (1 - f_0)$

$d^3\vec{k} = dk_x\, dk_y\, dk_z$

$$\int \tau v_x^2 \frac{\partial f_0}{\partial \varepsilon}\, d^3\vec{k} = \int v_x^2 \phi(\varepsilon)\, d^3\vec{k} = \int v_y^2 \phi(\varepsilon)\, d^3\vec{k} =$$

$$= \int v_z^2 \phi(\varepsilon)\, d^2\vec{k} = \frac{1}{3} \int v^2 \phi(\varepsilon)\, d^3\vec{k}$$

$(\varepsilon = \frac{1}{2} m (v_x^2 + v_y^2 + v_z^2) = \frac{1}{2} m v^2)$

$$j_x = \frac{e^2 n E_x}{k_B T} \cdot \frac{1}{3} \frac{\int_0^\infty v^2 \phi(\varepsilon)\, d^3\vec{k}}{\int f_0\, d^3\vec{k}} =$$

$$= \frac{1}{3} \frac{e^2 n E_x}{k_B T} \cdot \frac{\int_0^\infty \frac{2\varepsilon}{m_e^*} \phi(\varepsilon)\, 4\pi k^2 dk}{\int f_0\, 4\pi k^2 d\vec{k}} =$$

$$= \frac{2}{3} \frac{e^2 n E_x}{k_B T} \cdot \frac{\int_0^\infty \frac{\varepsilon}{m_e^*} \phi(\varepsilon)\, 4\pi k^2 dk}{\int_0^\infty f_0\, 4\pi k^2 dk}$$

$$4\pi k^2 dk = 4\pi \cdot \frac{2 m_e^* \varepsilon}{\hbar^2}\, dk$$

$$d\varepsilon = \frac{\hbar^2}{m_e^*} k\, dk = \frac{\hbar^2}{m_e^*} \frac{\sqrt{2 m_e^* \varepsilon}}{\hbar}\, dk$$

$$dk = \frac{m_e^*}{\hbar} \cdot \frac{1}{\sqrt{2 m_e^* \varepsilon}}\, d\varepsilon$$

$$\Rightarrow \quad 4\pi k^2 dk = \frac{8\pi m_e^* \varepsilon}{\hbar^3} \cdot m_e^* \cdot \frac{1}{\sqrt{2 m_e^* \varepsilon}}\, d\varepsilon =$$

$$= \frac{8\pi}{\hbar^3} \cdot \frac{1}{\sqrt{2}} \cdot m_e^{*3/2}\, \varepsilon^{1/2} d\varepsilon$$

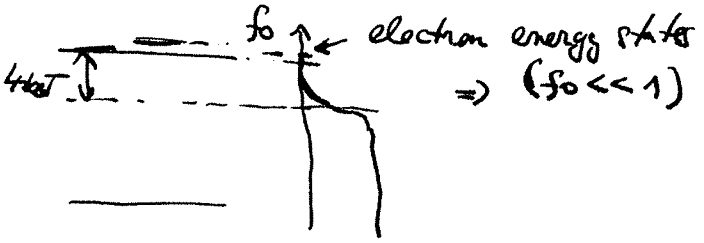
$$j_x = \frac{2}{3} \frac{e^2 n E_x}{k_B T m_e^*} \cdot \frac{\int_0^\infty \phi(\varepsilon)\, \varepsilon^{3/2} d\varepsilon}{\int_0^\infty \phi(\varepsilon)\, \varepsilon^{1/2} d\varepsilon} =$$

$$= \frac{2}{3} \frac{e^2 n E_x}{k_B T m_e^*} \frac{\int_0^\infty \tau f_0 (1 - f_0)\, \varepsilon^{3/2} d\varepsilon}{\int_0^\infty f_0\, \varepsilon^{1/2} d\varepsilon}$$

Now, let us suppose that the semiconductor is non-degenerate. Then $f_0 \ll 1$

(because for non degenerate semiconductors

$\varepsilon_F > -4k_BT$



Therefore $1-f_0 \approx 1$ $\left(f_0(1-f_0) = \underset{\text{small}}{f_0} - \underset{\text{very small}}{f_0^2} \right.$

$\Rightarrow$ j_x reduces to

$$j_x = \frac{2}{3}\,\frac{e^2 n E_x}{k_BT\, m_e^*}\,\frac{\int_0^\infty \tau f_0\, \varepsilon^{3/2} d\varepsilon}{\int_0^\infty f_0\, \varepsilon^{1/2} d\varepsilon}$$

Integration per-partes gives

$$\int_0^\infty \varepsilon^{3/2} f_0\, d\varepsilon = \frac{3}{2}\, k_BT \int_0^\infty \varepsilon^{1/2} d\varepsilon$$

$$\Rightarrow j_x = \frac{2}{3}\,\frac{e^2 n E_x}{k_BT\, m_e^*}\cdot k_BT \cdot \frac{3}{2}\,\frac{\int_0^\infty \tau f_0\, \varepsilon^{3/2} d\varepsilon}{\int_0^\infty f_0\, \varepsilon^{3/2} d\varepsilon} =$$

$$= \frac{e^2 n E_x}{m_e^*}\cdot \langle \tau \rangle \quad ; \text{ where } \langle \tau \rangle = \frac{\int_0^\infty \tau f_0\, \varepsilon^{3/2} d\varepsilon}{\int_0^\infty f_0\, \varepsilon^{3/2} d\varepsilon}$$

From previous calculations we know that

$$j_x = \rho_e v_x = (-e)\, n \underbrace{\langle v_x \rangle}_{\text{drift velocity}}$$

$$\Rightarrow j_x = \frac{(-e)\cdot(-e)\cdot n\, E_x}{m_e^*}\,\langle \tau \rangle = \overbrace{(-e)\, n}^{\rho_e} -\mu\, E_x$$

where $\mu = \frac{e}{m_e^*}\langle \tau \rangle$ is mobility

$$j_x = \rho_c \langle v_x \rangle = \rho_c \underbrace{(-\mu E_x)}_{\langle v_x \rangle} = (-ne)(-\mu)E_x = ne\mu E_x$$

ρ_c ... charge density $(-e)n$ for electrons

$+ep$ for holes

$$j_x = ne\mu E_x = \sigma E_x \qquad U = RI \qquad I = \frac{1}{R} \cdot U$$

$$\updownarrow \; j = \sigma \cdot E$$

σ ... electric conductivity

Equation above represents the Ohm's law

Solution of Boltzmann transport equation
(General case) - stationary

$$\vec{v}\cdot\nabla_{\vec{r}} f - \frac{e}{\hbar}\left[\vec{E}+\vec{v}\times\vec{B}\right]\nabla_{\vec{k}} f = -\frac{f_1}{\tau} = -\frac{(f-f_0)}{\tau}$$

$$f_1 = -\left(\frac{\partial f_0}{\partial \varepsilon}\right)\vec{\chi}\cdot\vec{E} \qquad \vec{\chi} = \frac{\hbar\Delta\vec{k}}{m^*}$$

We are looking for f_1 with the precision to the 1. st term of Taylor expansion (small deviations)

We calculate $\nabla_{\vec{r}} f_0$; $\nabla_{\vec{r}} f_1$, $\nabla_{\vec{k}} f_0$, $\nabla_{\vec{k}} f_1$ and perform linearization (1. st term in $\vec{E}$)

⇒ This leads to equation

$$\vec{\chi} = \vec{a} + \vec{b}\,\vec{\chi}$$

We introduce $\vec{\chi}^* = -\frac{m^*}{\hbar e}\vec{\chi}$; $\mu = \frac{e}{m^*}$

⇒ Solution of the equation is

$$\vec{\chi}^* = \frac{\tau\vec{P} + \mu\tau^2\left[\vec{B}\times\vec{P}\right] + \mu^2\tau^3(\vec{B}\cdot\vec{P})\vec{B}}{1+\mu\tau B^2}$$

$$\vec{P} = \frac{k_B}{e}(x-\eta)\nabla_{\vec{r}}T + \frac{k_B T}{e}\nabla_{\vec{r}}\eta - \nabla_{\vec{r}}\varphi$$

$$x = \frac{\varepsilon}{k_B T} \qquad \eta = \frac{\varepsilon_F}{k_B T}$$

For $\vec{B} = 0$ we have $\vec{\chi}^* = \tau\vec{P}$

The density of electric current and the density of energy flux

$\vec{J} = \sum_{\vec{k}} \frac{2}{V} f(\vec{k},\vec{r},t)\vec{v}$ .. density of flux of particles

$\vec{j}_e = -\frac{2e}{V} \sum_{\vec{k}} f(\vec{k},\vec{r},t)\vec{v}$ the density of electric current (electronic)

$\vec{v} = \frac{\hbar\vec{k}}{m_e^*}$

$$\vec{j}_e = -\frac{2e}{V} \frac{\int f(\vec{k},\vec{r},t)\,\vec{v}\,d^3\vec{k}}{\frac{(2\pi)^3}{V}}$$

Volume on 1 state of the k-space

$$\vec{j}_e = -\frac{e\hbar}{4\pi^3 m_e^*} \int f(\vec{k},\vec{r},t)\,\vec{k}\cdot d^3\vec{k}$$

kinetic energy

potential energy

$$\vec{w}_e = \sum_{\vec{k}} \frac{2}{V} f(\vec{k},\vec{r},t)\,\vec{v}\,(\varepsilon - e\varphi)$$

$\downarrow$

$$\vec{w}_e = \frac{\hbar}{4\pi^3 m_e^*} \int f(\vec{k},\vec{r},t)(\varepsilon - e\varphi)\,\vec{k}\cdot d^3\vec{k}$$

$f = f_0 + f_1$ $\quad \int \underset{\uparrow}{f_0(\vec{k})}\,\vec{k}\,d^3\vec{k} = 0$

even function

Then

$$\vec{j}_e = -\frac{e\hbar}{4\pi^3 m_e^*} \int \left(-\frac{\partial f_0}{\partial \varepsilon}\right) \vec{\chi}\cdot\vec{k}\cdot d^3\vec{k}$$

We integrate in spherical coordinates, introduce

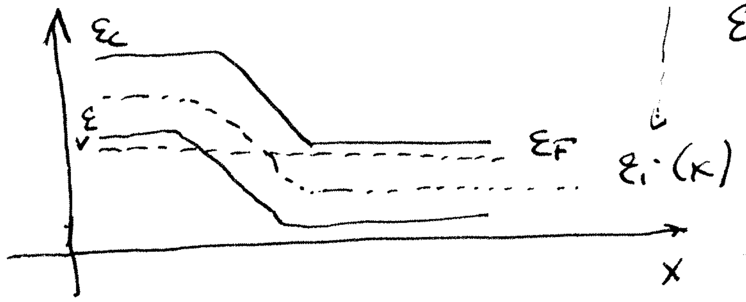
$$\langle \chi^* \rangle = \frac{\int_0^\infty -\left(\frac{\partial f_0}{\partial \varepsilon}\right)\vec{\chi}^*\, \varepsilon^{3/2}\, d\varepsilon}{\int_0^\infty \left(-\frac{\partial f_0}{\partial \varepsilon}\right)\varepsilon^{3/2}\, d\varepsilon}$$

We will from this point assume, that magnetic field vector $\vec{B} \parallel z$.

We obtain after some calculations

$$\vec{j}_e = \frac{e^2 n}{m_e^*}\langle \vec{\chi}^* \rangle = \overleftrightarrow{\sigma}\, \nabla_{\vec{r}} \frac{\varepsilon_F(\vec{r})}{e} + \overleftrightarrow{\beta}\, \nabla_{\vec{r}} T$$

Inhomogeneous semiconductor



$$\varepsilon_F = \varepsilon_i + k_B T \ln \frac{n}{n_i}$$

Intrinsic Fermi energy

$$\overleftrightarrow{\sigma} = \begin{pmatrix} \sigma_{xx} & -\sigma_{xy} & 0 \\ \sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix} \qquad \vec{B} \parallel z$$

$$\overleftrightarrow{\beta} = \begin{pmatrix} -\beta_{xx} & \beta_{xy} & 0 \\ -\beta_{xy} & -\beta_{xx} & 0 \\ 0 & 0 & \beta_{zz} \end{pmatrix}$$

We repeat the last figure from the previous lecture and explain its meaning.

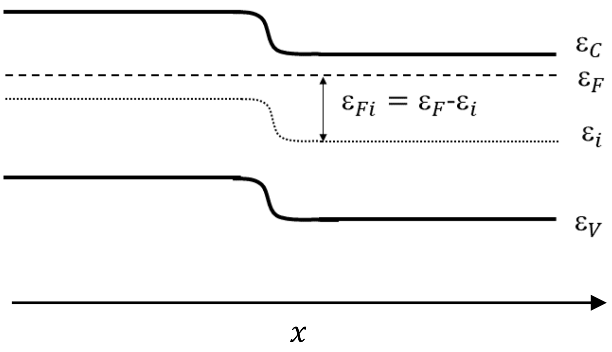


Figure – an example of the spatial profile of bands in an inhomogeneous semiconductor. Here ε_F is the Fermi energy and ε_i is the intrinsic Fermi energy. Their difference ε_{Fi} characterizes the spatial changes.

The concentration of electrons (non –degenerate case) is

$$n(\boldsymbol{r}) = N_C e^{\frac{\varepsilon_F}{k_B T}}$$

The intrinsic concentration is

$$n_i = N_C e^{\frac{\varepsilon_i}{k_B T}}$$

We can write

$$N_C = n_i e^{-\frac{\varepsilon_i}{k_B T}}$$

$$n(\boldsymbol{r}) = n_i e^{\frac{\varepsilon_F - \varepsilon_i}{k_B T}}, \qquad \varepsilon_F - \varepsilon_i = k_B T(\boldsymbol{r}) ln \frac{n(r)}{n_i} = \varepsilon_{Fi}$$

$$\nabla_{\boldsymbol{r}} \varepsilon_{Fi} = k_B \nabla_{\boldsymbol{r}} T \; ln \frac{n(\boldsymbol{r})}{n_i} + k_B T \nabla_r \; ln \frac{n(\boldsymbol{r})}{n_i} = k_B \nabla_{\boldsymbol{r}} T \; ln \frac{n(\boldsymbol{r})}{n_i} + k_B T \frac{\nabla_{\boldsymbol{r}} n(\boldsymbol{r})}{n(\boldsymbol{r})}$$

The intrinsic Fermi energy ε_{Fi} can be written using the potential as $\varepsilon_{Fi} = -e\varphi_i$. Then the corresponding electric field is

$$\boldsymbol{E}_i = -\nabla_{\boldsymbol{r}} \varphi_i = \frac{\nabla_r \varepsilon_{Fi}}{e}.$$

The total electric field $\boldsymbol{E}^*$ in the sample is a sum of the electric field $\boldsymbol{E} = -\nabla_{\boldsymbol{r}} \varphi$ formed as a result of the application of external bias and the electric field $\boldsymbol{E}_i$ formed due to the gradient of concentration of electrons (or holes).

$$\boldsymbol{E}^* = \boldsymbol{E} + \boldsymbol{E}_i$$

The solution of the Boltzmann transport equation leads to the equation for the density of the electric current

$$\boldsymbol{j} = \overleftrightarrow{\sigma}\boldsymbol{E}^{*} + \overleftrightarrow{\beta}_{0}\nabla_{\boldsymbol{r}}T,$$

Which can be written as

$$\boldsymbol{j} = \overleftrightarrow{\sigma}\boldsymbol{E} + \overleftrightarrow{\sigma}\frac{k_B T}{e}\frac{\nabla_r n(\boldsymbol{r})}{n(\boldsymbol{r})} + \frac{k_B}{e} ln \frac{n(\boldsymbol{r})}{n_i}\nabla_{\boldsymbol{r}}T + \overleftrightarrow{\beta}_{0}\nabla_{\boldsymbol{r}}T.$$

We define a new tensor $\overleftrightarrow{\beta}$ combining the 3rd and 4th term of the equation and obtain the drift-diffusion equation

$$\boldsymbol{j} = \overleftrightarrow{\sigma}\boldsymbol{E} + \overleftrightarrow{\sigma}\frac{k_B T}{e}\frac{\nabla_{\boldsymbol{r}} n(\boldsymbol{r})}{n(\boldsymbol{r})} + \overleftrightarrow{\beta}\nabla_{\boldsymbol{r}}T$$

The first term represents the electric current caused by externally applied bias (drift term), the second term is the electric current due to diffusion of carriers caused by the concentration gradient and the third term is the electric current caused by gradient of temperature.

Here $$\overleftrightarrow{\sigma} = \begin{pmatrix} \sigma_{xx} & -\sigma_{xy} & 0 \\ \sigma_{xy} & \sigma_{xx} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$

$$\sigma_{xx} = \frac{e^2 n}{m_e^*} \left\langle \frac{\tau}{1+b^2} \right\rangle \qquad \sigma_{xy} = \frac{e^2 n}{m_e^*} \left\langle \frac{\tau b}{1+b^2} \right\rangle$$

$$\sigma_{zz} = \frac{e^2 n}{m_e^*} \langle \tau \rangle \qquad b = \frac{e}{m_e^*} \tau B = \gamma \tau B$$

$$\overleftrightarrow{\beta} = \begin{pmatrix} -\beta_{xx} & \beta_{xy} & 0 \\ -\beta_{xy} & -\beta_{xx} & 0 \\ 0 & 0 & -\beta_{zz} \end{pmatrix}$$

$$\beta_{xx} = -\frac{e n k_B}{m_e^*} \left\langle \frac{\tau (x-\eta)}{1+b^2} \right\rangle$$

$$\beta_{xy} = -\frac{e n k_B}{m_e^*} \left\langle \frac{\tau b (x-\eta)}{1+b^2} \right\rangle$$

$$\beta_{zz} = \frac{e n k_B}{m_e^*} \langle \tau (x-\eta) \rangle$$

Transition relations to holes

$-e \to +e \qquad \eta \to \eta' \qquad x \to x' \qquad b \to b_h$

$$b_h = \frac{e}{m_h^*} \tau B$$

With the same approach it is possible to derive the equation for heat transfer

$$\vec{w} = T \overleftrightarrow{\beta} \vec{E} + \overleftrightarrow{\chi} \nabla T$$

$$\overleftrightarrow{\kappa} = \overleftrightarrow{\kappa}_e + \overleftrightarrow{\kappa}_\varphi$$

$\overleftrightarrow{\kappa}_\varphi$ ... diagonal matrix describes the thermal conductivity of lattice

$$\overleftrightarrow{\kappa} = \begin{pmatrix} -\kappa_{xx} - \kappa_\varphi & \kappa_{xy} & 0 \\ -\kappa_{xy} & -\kappa_{yy} - \kappa_\varphi & 0 \\ 0 & 0 & -\kappa_{zz} - \kappa_\varphi \end{pmatrix}$$

If both electrons and holes are present the following equations are valid

$$\vec{j} = \vec{j}_e + \vec{j}_h \qquad \vec{w} = \vec{w}_e + \vec{w}_h$$

The equations for $\vec{j}$ and $\vec{w}$ can be re-formulated

$$\vec{j} = \overleftrightarrow{\sigma} \vec{E}^{*} + \overleftrightarrow{\beta} \nabla_{\vec{r}} T$$

$$\vec{w} = T \overleftrightarrow{\beta} . \vec{E}^{*} + \overleftrightarrow{\kappa} \nabla_{\vec{r}} T$$

$\vec{I}$ .. unit tensor

$$\overleftrightarrow{\sigma} \vec{E}^{*} = \vec{j} - \overleftrightarrow{\beta} \nabla_{\vec{r}} T \qquad / . \overleftrightarrow{\sigma}^{-1}$$

$$\vec{E}^{*} = \underbrace{\overleftrightarrow{\sigma}^{-1}}_{\overleftrightarrow{\rho}} \vec{j} - \underbrace{\overleftrightarrow{\sigma}^{-1} \overleftrightarrow{\beta}}_{\overleftrightarrow{\alpha}} \nabla_{\vec{r}} T \qquad \overleftrightarrow{\sigma}^{-1} \equiv \overleftrightarrow{\rho}$$

$$\overleftrightarrow{\alpha} = \overleftrightarrow{\sigma}^{-1} . \overleftrightarrow{\beta}$$

$\overleftrightarrow{\rho}$ ... resistivity tensor

$\overleftrightarrow{\alpha}$ .. Seebeck coefficient

$$\vec{w} = T\overleftrightarrow{\beta}\left(\overleftrightarrow{\rho}\vec{j} - \overleftrightarrow{\alpha}\nabla_{\vec{r}}T\right) + \overleftrightarrow{\varkappa}\nabla_{\vec{r}}T$$

$$\vec{w} = \underbrace{T\underbrace{\overleftrightarrow{\beta}\overleftrightarrow{\rho}}_{\overleftrightarrow{\alpha}}}_{\overleftrightarrow{\Pi}}\vec{j} + \overbrace{\left(-T\overleftrightarrow{\beta}\overleftrightarrow{\alpha} + \overleftrightarrow{\varkappa}\right)}^{\overleftrightarrow{\lambda}}\nabla_{\vec{r}}T$$

$\overleftrightarrow{\Pi} = \overleftrightarrow{\alpha}T$ Bridgman relation

$\overleftrightarrow{\Pi}$ .. Peltier coefficient

$\overleftrightarrow{\lambda}$ .. thermal conductivity

$$\overleftrightarrow{\rho} = \begin{pmatrix} \rho_{xx} & +\rho_{xy} & 0 \\ -\rho_{xy} & \rho_{yy} & 0 \\ 0 & 0 & \rho_{zz} \end{pmatrix} \qquad \rho_{xx} = \rho_{yy}$$

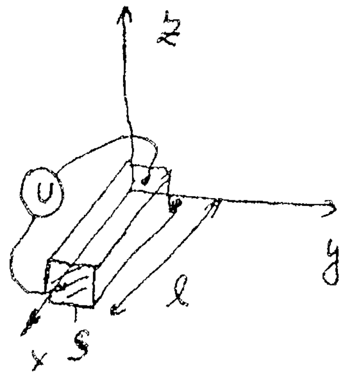
$$\overleftrightarrow{\alpha} = \begin{pmatrix} \alpha_{xx} & \alpha_{xy} & 0 \\ -\alpha_{xy} & \alpha_{yy} & 0 \\ 0 & 0 & \alpha_{zz} \end{pmatrix} \qquad \alpha_{xx} = \alpha_{yy}$$

$$\overleftrightarrow{\Pi} = \begin{pmatrix} \Pi_{xx} & \Pi_{xy} & 0 \\ -\Pi_{xy} & \Pi_{yy} & 0 \\ 0 & 0 & \Pi_{zz} \end{pmatrix} \qquad \Pi_{xx} = \Pi_{yy}$$

$$\overleftrightarrow{\lambda} = \begin{pmatrix} -\lambda_{xx} & \lambda_{xy} & 0 \\ -\lambda_{xy} & -\lambda_{yy} & 0 \\ 0 & 0 & -\lambda_{zz} \end{pmatrix} \qquad \lambda_{xx} = \lambda_{yy}$$

Transport effects without $\vec{B}$

Ohm's law : Theory :



$\vec{E} = (E,0,0)$ E - field due to applied bias

$\vec{B} = (0,0,0)$

$\Rightarrow b = 0$

$\vec{E}^* = \vec{E}$

$$\vec{j} = \overleftrightarrow{\sigma}\,\vec{E}$$

$$j_x = \sigma_{xx}(0)\cdot E_x = \underbrace{\frac{e^2 n}{m_e^*}\langle\tau\rangle}_{\sigma_{xx}(0)\,\equiv\,\sigma_0} E_x \qquad j = \sigma_0 E$$

$$R = \frac{U}{I} = \rho_0 \cdot \frac{l}{S} \Rightarrow \rho_0 = \frac{U}{I}\cdot\frac{S}{l}$$

$$\frac{I}{S} = \frac{1}{\rho_0}\cdot\frac{U}{l}$$

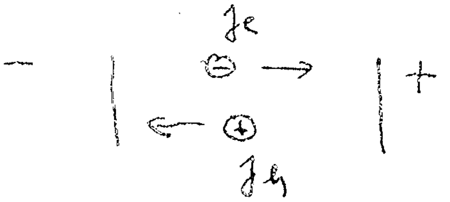
$$\downarrow$$

$$j = \frac{1}{\rho_0}\cdot E = \sigma_0\cdot E$$

$\Rightarrow$ σ_0 from experiment equals $\frac{e^2}{m_e^*}\cdot n\,\langle\tau\rangle$

Because $\sigma_0 \sim e^2$ electrons and holes contribute to electric current

$$\vec{j} = \vec{j}_e + \vec{j}_h = \left(\frac{e^2 n}{m_e^*}\langle\tau_e\rangle + \frac{e^2 p}{m_h^*}\langle\tau_h\rangle\right)\vec{E}$$



Thermal conductivity

Thermal conductivity of material consists of thermal conductivity of electrons (holes) which we derived from BTE and thermal conductivity of lattice, which is added to the formulas

$\vec{j} = (0, 0, 0)$

$\vec{B} = (0, 0, 0)$

$\nabla_{\vec{r}} T = (\nabla_x T, 0, 0)$

$$\vec{W} = \overleftrightarrow{\lambda}\, \nabla_{\vec{r}} T$$

$$W_x = -\lambda_{xx} \nabla_x T$$

$$W_x = -\left[\varkappa_{xx}(0) + \varkappa_\varphi - T \beta_{xx}(0)\, \alpha_{xx}(0)\right] \nabla_x T$$

$$W_x = -\left[\varkappa_{xx}(0) + \varkappa_\varphi - T \frac{\beta_{xx}^2(0)}{\sigma_{xx}(0)}\right] \nabla_x T$$

$$W_x = -\left[\varkappa_{xx}(0) - T \cdot \frac{\beta_{xx}^2(0)}{\sigma_{xx}(0)}\right] \nabla_x T - \varkappa_\varphi \nabla_x T$$

After applying formulas for $\varkappa_{xx}(0)$, $\beta_{xx}(0)$ and $\sigma_{xx}(0)$ we obtain

$$W_x = \left[L \cdot \sigma_{xx}(0) \cdot T - \varkappa_\varphi\right] \nabla_x T$$

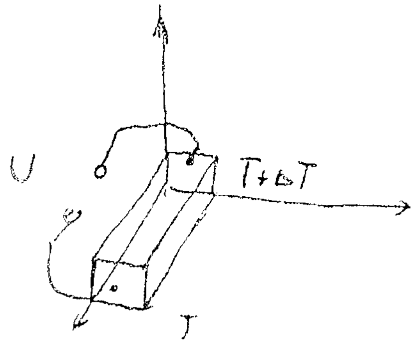
$$L = \left(\frac{k_B}{e}\right)^2 \left(\langle \tau x^2 \rangle - \frac{\langle \tau x \rangle^2}{\langle \tau \rangle}\right) \qquad x = \frac{\varepsilon}{k_B T}$$

$L \equiv$ Lorentz number

$$\varkappa_{xx} = \frac{n k_B T}{m_e^*} \left\langle \frac{\tau (x-3)^2}{1+b2} \right\rangle \qquad \varkappa_{xy} = \frac{k_B T n}{m_e^*} \left\langle \frac{\tau (x-3)^2 b}{1+b2} \right\rangle$$

Thermoelectric (Seebeck) effect

The Seebeck effect was discovered in 1821 by german physicist Thomas Seebeck (born in Tallin, graduated in Göttingen).



U ... open circuit voltage formed by Seebeck effect due to a temperature gradient in the sample.

$U = \alpha \cdot \Delta T$ (experiment)

$$j^x = \sigma_{xx}(0)\, E_x^* - \beta_{xx}(0)\, \nabla_x T = 0 \quad \text{(open circuit)}$$

$$E_x^* = \underbrace{\frac{\beta_{xx}(0)}{\sigma_{xx}(0)}}_{\alpha_{xx}(0)} \nabla_x T \qquad -\nabla_x \varphi^* = \alpha_{xx}(0) \cdot \nabla_x T$$

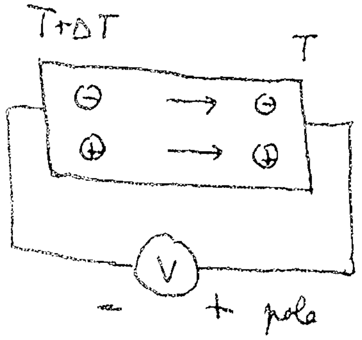
$\nearrow$ Seebeck coefficient

Using the Seebeck effect it is possible the type of the semiconductor

$\sigma_{xx}(0) \sim e^2$ $\qquad$ $\beta_{xx}(0) \sim (-e)$

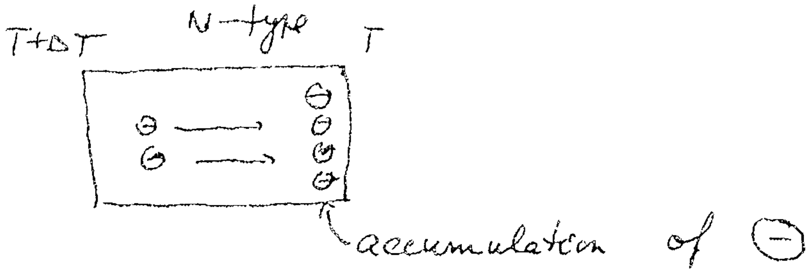
↓ the same for electrons $(-e)$ and holes $(+e)$

↓ different for electrons and holes



Electrons and holes diffuse against the temperature gradient.

If the semiconductor is n-type, the diffusion of electrons will cause decrease of the potential on the (+) end that is at lower T. (negative charge is built on the cooler end to stop the flow of electrons from the hotter end.

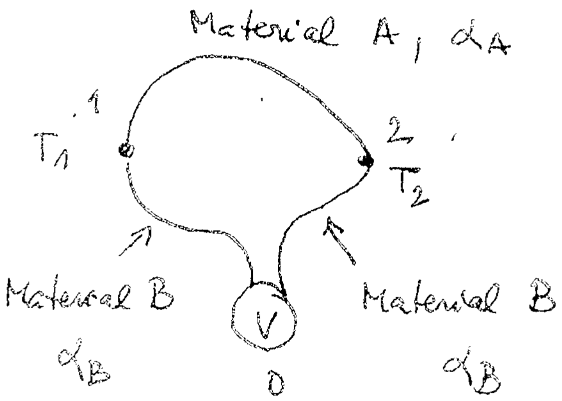


In case of P-type semiconductor the situation is opposite.

Another application of Seebeck effect
– the thermocouple

Thermocouple is formed from two materials with different Seebeck coefficients.

It is used to measure temperature difference, or absolute temperature.



The bias measured by the voltmeter

$$U = \int_1^2 E_A \, dx + \int_2^0 E_B \, dx + \int_0^1 E_B \, dx =$$

$$= \int_1^2 E_A \, dx + \int_2^1 E_B \, dx = \int_1^2 (E_A - E_B) \, dx$$

$$= \int_{T_1}^{T_2} (\alpha_A - \alpha_B) \cdot \frac{dT}{dx} \, dx = (\alpha_A - \alpha_B)(T_2 - T_1)$$

α_A, α_B .. Seebeck coefficients of materials A and B

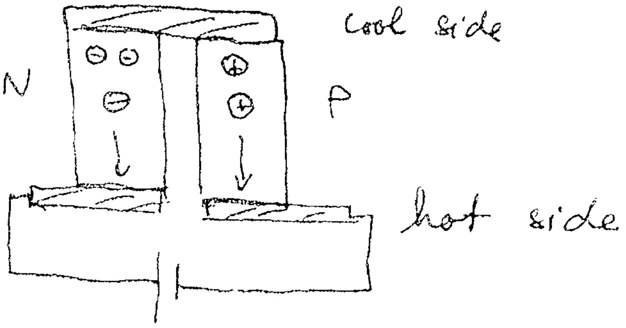
Normally we fix T_1 (mixture of ice and water, nitrogen, helium)

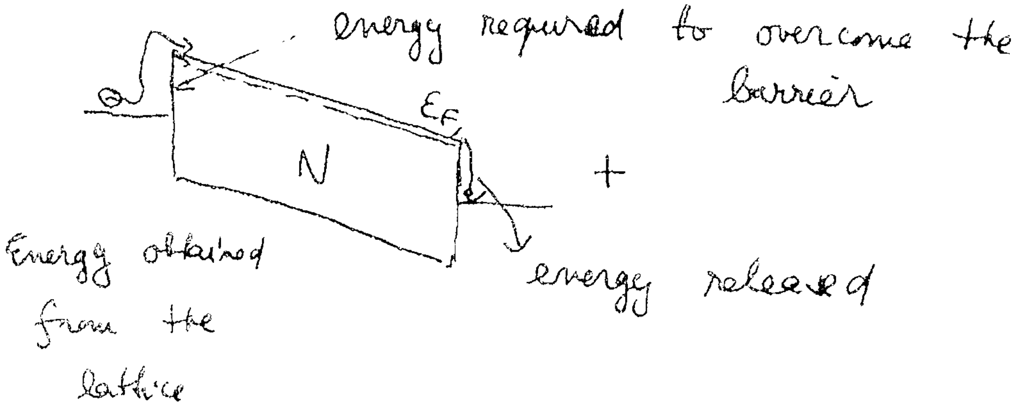
and knowing α_A and α_B we calculate T_2

Peltier effect

Peltier effect consists of formation of temperature gradient as a result of flow of electric current.

$$W_x = \Pi_{xx} j_x$$





= cooling

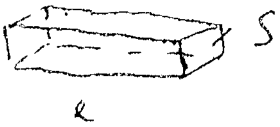
When we reverse the direction of the electric current, the hot and cold sides exchange

Calculation of efficiency of the Peltier element

$$W_x = \underset{\uparrow}{\Pi_{xx}}\, j_x + \lambda_{xx} \underset{\nwarrow}{\nabla_x} T$$

Primary effect - $j_x \to \nabla_x T$

Secondary effect
The gradient due to current flow results in opposit flow of carriers



$$R = \rho \cdot \frac{l}{S} = \frac{U}{I}$$

$$U = \frac{\rho l I}{S} = \rho l j$$

$$\frac{U}{l} = \rho \cdot j \qquad E = \rho \cdot j$$

$$E = \frac{1}{\sigma} j \qquad j = \sigma E$$

$$\frac{\Pi \cdot j}{\lambda \nabla_x T} = \frac{\alpha T j}{\lambda \nabla_x T} = \frac{\alpha T \cdot \sigma \cdot \frac{U}{l}}{\lambda \cdot \frac{\Delta T}{l}} =$$

$$= \frac{\alpha^2 T \cdot \sigma U}{\lambda \cdot \underbrace{\alpha \Delta T}_{\text{Seebeck voltage } U_T}} = \frac{\alpha^2 \sigma}{\lambda} \cdot T \cdot \frac{U}{U_T} = Z \cdot T \cdot \frac{U}{U_T}$$

$$Z = \frac{\alpha^2 \sigma}{\lambda}$$

For a high efficiency of the effect Z must be high, high α and σ, low λ

Drift-diffusion equation – introduction of mobility and diffusion coefficient

$$\vec{j} = \overleftrightarrow{\sigma}\vec{E} + \overleftrightarrow{\sigma}\,\frac{k_BT}{e}\cdot\frac{\nabla_{\vec{r}}\, n(\vec{r})}{n} + \overleftrightarrow{\beta}\,\nabla_{\vec{r}}T$$

assuming $\nabla_{\vec{r}}T$ we can calculate in the absence of magnetic field ($\vec{B}=0$)

$$j_x = \sigma_{xx}E_x + \sigma_{xx}\frac{k_BT}{e}\cdot\frac{dn(x)}{dx}\cdot\frac{1}{n}$$

$$\sigma_{xx} = \frac{e^2 n}{m_x^*}\langle\tau\rangle = e\cdot n\cdot\mu_e$$

where $\mu_e = \frac{e}{m_x^*}\langle\tau\rangle$ we call „mobility“

$$j_x = en\mu_eE_x + \frac{en\mu_e k_BT}{e}\cdot\frac{1}{n}\cdot\frac{dn(x)}{dx} =$$

$$= en\mu_eE_x + \mu_e k_BT\frac{dn(x)}{dx} =$$

$$= en\mu_eE_x + eD_e\frac{dn(x)}{dx}$$

$D_e = \frac{k_BT}{e}\cdot\mu_e$ .. we call „diffusion constant“

Transport effects in magnetic field

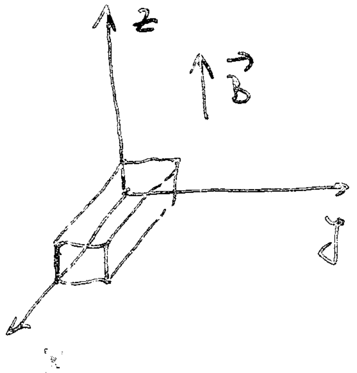
If the deviation from equilibrium in the sample is small (condition under which we solved the Boltzmann transport equation), then all „zz" elements of the transport tensors are not a function of $\vec{B}$ (i.e. „b" in the eqs.)

⇒ all the transport effects ∥ to „z" direction do not depend on $\vec{B}$ (e.g. $j_z = \sigma_{zz} E_z \neq f(\vec{B})$)

On $\vec{B}$ depend therefore only transversal effects (i.e. when $\vec{B}$ is perpendicular to the acting forces)

$$\sigma_{zz} = \frac{e^2 n}{m_e^*}\langle\tau\rangle$$

Transversal magnetoresistance



$$\vec{E} = \vec{\rho}\,\vec{j} \qquad \vec{j} = (j_x, 0, 0)$$

$$\vec{B} = (0, 0, B)$$

$$E_x = \rho_{xx}\, j_x \qquad \rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2}$$

$$\rho_{xx}(0) = \frac{1}{\sigma_{xx}(0)}$$

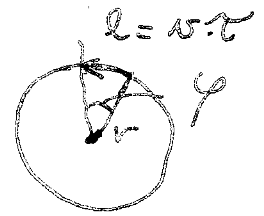
$$\Delta\rho(B) = \rho_{xx}(B) - \rho_{xx}(0) = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2} - \frac{1}{\sigma_{xx}(0)}$$

$$\sigma_{xx} = \frac{e^2 n}{m_e^*}\left\langle \frac{\tau}{1+b^2} \right\rangle \qquad \sigma_{xy} = \frac{e^2 n}{m_e^*} \cdot \left\langle \frac{\tau b}{1+b^2} \right\rangle$$

$$b = \frac{e}{m^*}\tau B =$$
$$= \mu_n \tau B$$

Microscopic explanation

If magnetic field is applied perpendicular to the sample then electrons in the sample start to move ~~in~~ circles



$$\frac{m_e^* v^2}{r} = evB$$

repulsive force

Lorentz force

$l = v\tau$ mean free path

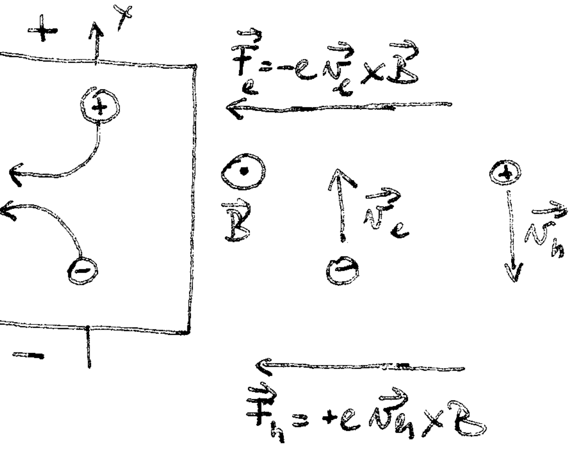
$$tg\,\varphi \approx \varphi = \frac{l}{r} = \frac{v\tau\cdot eB}{m_e^* v} = \underbrace{\left(\frac{e}{m_e^*}\cdot\tau\right)}_{\mu_e} B$$

φ = „rotation angle"

μ_e mobility of electrons

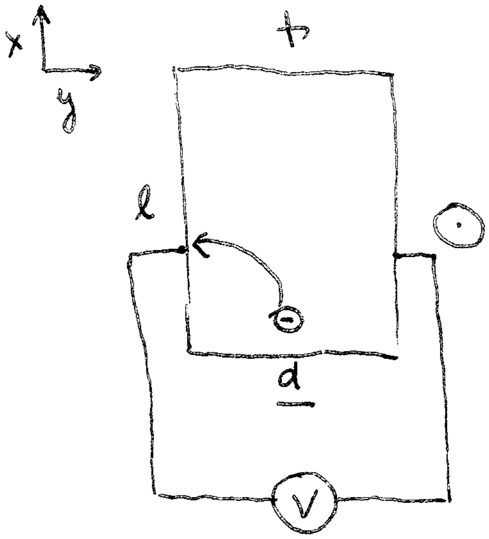
The angle φ does not depend on velocity, it depends only on the ratio $\frac{\tau}{m_e^*}$

(analogically for holes)



The Lorentz force deflects both electrons and holes in the same direction, perpendicular to velocity and $\vec{B}$

Let us now focus e.g. on N-type semiconductor (electrons are majority carriers)



Electrons drifting from the cathode to the anode are deflected by the Lorentz force and accumulated on the left side of the sample

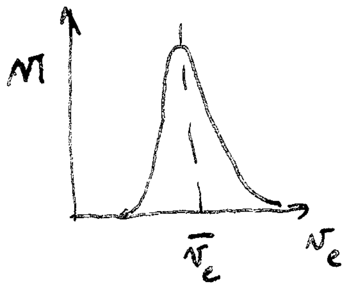
⇒ transversal electric field E_y is formed (Hall voltage U_H can be measured)

$$V_y \equiv U_H = \frac{E_y}{d}$$

The E-field E_y compensates the action of the Lorentz field, in this quasiequilibrium electrons with velocity $\bar{v}_e$ are no more deflected and drift directly from the cathode to the anode

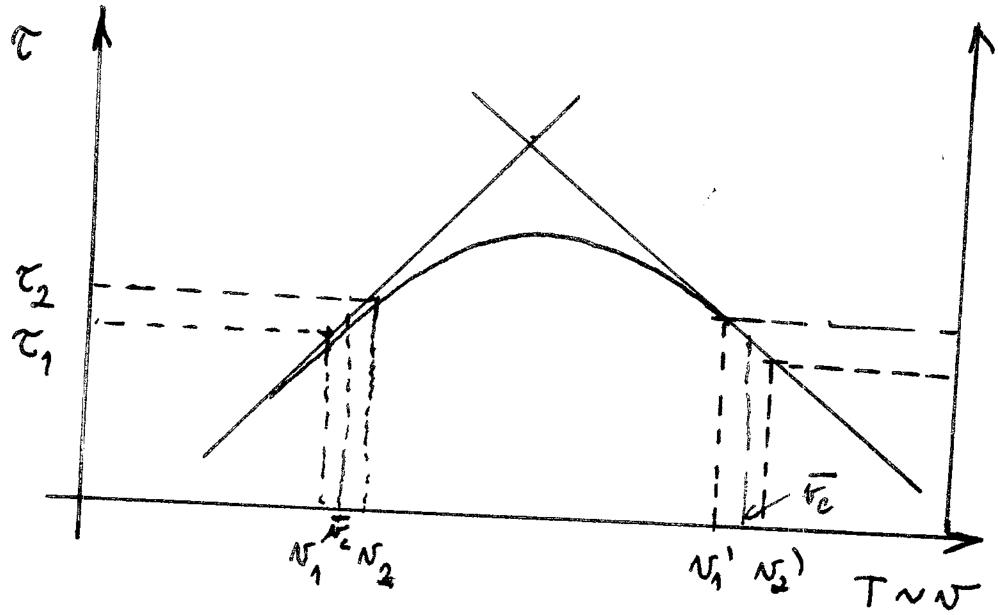
$$eE_y = e\bar{v}_e B \Rightarrow \bar{v}_e = \frac{E_y}{B}$$

However, the electrons in the material have a certain distribution of velocities

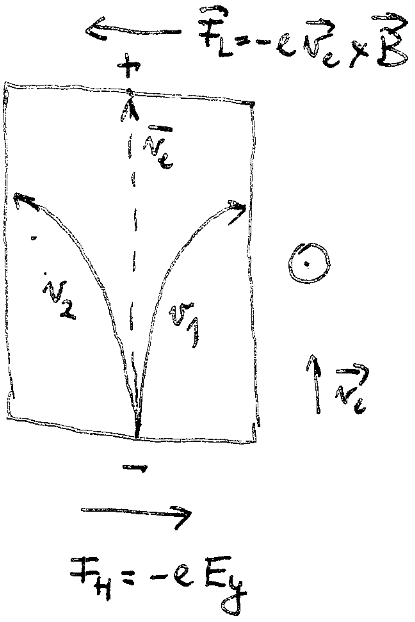


The previos equation holds only for electrons with velocity $\bar{v}_e$. Electrons with $v_e < \bar{v}_e$ and $v_e > \bar{v}_e$ are deflected to both sides.

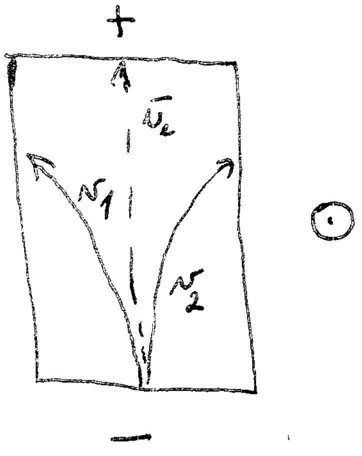
Different velocities correspond to different relaxation times τ (and different rotation angles φ) in dependence of temperature.



At low T (scattering on ionized impurities, v_2 electrons (higher T) have a larger τ and larger φ than v_1 electrons. The transversal Hall force $(-eE_y)$ compensates exactly action of the Lorentz force $(-e v.B)$ for $\bar{v}_e$ electrons with $\tau = \bar{\tau}$ $(\varphi = \bar{\varphi})$. Both v_2 and v_1 electrons are deflected from direct path (in the „x" direction) v_2 electrons scatter less than $\bar{v}_e$ electrons, $\varphi_2 > \bar{\varphi}$, v_2 electrons are deflected to the left. v_1 electrons scatter more than $\bar{v}_e$ electrons, $\varphi_1 < \bar{\varphi}$, v_1 el. are deflected to the right. At high T (scattering on phonons, the situation is reversed.



low T



high T

In both cases the paths of electrons with $v \neq \bar{v}_e$ is longer than the path of $\bar{v}_e$ electrons This results in the higher resistivity in magnetic field

$$\rho(B) > \rho(0)$$

The Hall effect

One of the most important transverse effects in the magnetic field

$\vec{B} = (0, 0, B)$

$\vec{j} = (j_x, 0, 0)$

$\nabla_{\vec{r}} T = (0, 0, 0)$

$\vec{E} = \overleftrightarrow{\rho}\, \vec{j}$ .. $E_x = \rho_{xx} j_x$ (standard resistivity in magnetic field

$$E_y = -\rho_{xy} j_x$$

The experimentally observed transverse electric field depends on the electic current flowing in the „x" direction and the magnetic field in „z" direction.

Experiment: $E_y = R_H j_x B$

From our model is clear that

$$E_y = -\rho_{xy} j_x \Rightarrow R_H = -\frac{\rho_{xy}}{B}$$

After including the relations for ρ_{xy} we have

$$R_H = -\frac{\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2} \cdot \frac{1}{B} = -\frac{m_e^*}{e^2 n} \cdot \frac{1}{D} \cdot \frac{1}{B} \cdot \left\langle \frac{\tau b}{1+b^2} \right\rangle$$

$$D = \left\langle \frac{\tau}{1+b^2} \right\rangle + \left\langle \frac{\tau b}{1+b^2} \right\rangle$$

We can write R_H as

$$R_H = -\frac{r_H^{(e)}}{en} \qquad r_H^{(e)} = +\frac{1}{e} \cdot \frac{m_e^*}{D} \cdot \frac{1}{B} \cdot \left\langle \frac{\tau b}{1+b^2} \right\rangle$$

$r_H^{(e)}$ is called Hall scattering factor (for electrons)

$r_H^{(e)} \approx 1$ in many cases

Let us define the Hall mobility

$$\mu_H = r_H^{(e)} \cdot \mu_e = \frac{r_H}{en} \cdot en\mu = |R_H| \sigma_e$$

$$E_y = R_H j_x \cdot B = \frac{U_H}{d} \Rightarrow U_H = R_H \cdot j_x B \cdot d = R_H \sigma_e E_x \cdot B \cdot d =$$

$$= \mu_H \cdot \frac{U_x}{l} \cdot B \cdot d \quad ; \quad R_H = \frac{U_H}{\sigma_e E_x B \cdot d} = \frac{U_H l}{\sigma_e U_x B \cdot d}$$

From the measured R_H we can calculate concentration of carriers

$$R_H = -\frac{r_H^{(e)}}{e \cdot n} \quad \text{(N-type)} \qquad R_H = \frac{r_H^{(h)}}{ep}$$

$$n = -\frac{r_H^{(e)}}{eR_H} \qquad p = \frac{r_H^{(h)}}{eR_H}$$

Hall effect for two types of carriers

$$R_H = -\frac{1}{B} \cdot \frac{\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2} \qquad \ldots \text{ 1 type}$$

$$R_H = -\frac{1}{B} \frac{\sigma_{xy}^{(1)} + \sigma_{xy}^{(2)}}{(\sigma_{xx}^{(1)} + \sigma_{xx}^{(2)})^2 + (\sigma_{xy}^{(1)} + \sigma_{xy}^{(2)})^2}$$

Let us use an abbreviation

$$R_1 = -\frac{1}{B} \cdot \frac{\sigma_{xy}^{(1)}}{(\sigma_{xx}^{(1)} + \sigma_{xy}^{(1)})^2} \qquad R_2 = -\frac{1}{B} \frac{\sigma_{xy}^{(2)}}{(\sigma_{xy}^{(2)} + \sigma_{xx}^{(2)})^2}$$

$$\sigma_1 = \frac{\sigma_{xx}^{(1)2} + \sigma_{xy}^{(1)2}}{\sigma_{xx}^{(1)}} \qquad \sigma_2 = \frac{\sigma_{xx}^{(2)2} + \sigma_{xy}^{(2)2}}{\sigma_{xx}^{(2)}}$$

$\downarrow$

$$R = \frac{1}{D_0} \left[R_1 \sigma_1^2 + R_2 \sigma_2^2 + B^2 R_1 R_2 \sigma_1^2 \sigma_2^2 (R_1 + R_2) \right]$$

$$D_0 = (\sigma_1 + \sigma_2)^2 + B^2 \sigma_1^2 \sigma_2^2 (R_1 + R_2)^2$$

For weak B we can write

$$R = \frac{R_1 \sigma_1^2 + R_2 \sigma_2^2}{(\sigma_1 + \sigma_2)^2}$$

The above written equations are general, i.e. they are valid if the two types are , electrons and holes or e.g. two types of electrons with a different effective mass

For the case of electrons and holes we can write

$$R_1 = R_e = \frac{-v_H^{(e)}}{ne} \qquad R_2 = R_h = \frac{v_H^{(h)}}{pe}$$

$$\sigma_1 = ne\mu_e \qquad \sigma_2 = ep\mu_h$$

$$R_H = \frac{-\frac{v_H^{(e)}}{ne} n^2e^2\mu_e^2 + \frac{v_H^{(h)}}{pe} \cdot p^2e^2\mu_h^2}{(ne\mu_e + pe\mu_h)^2}$$

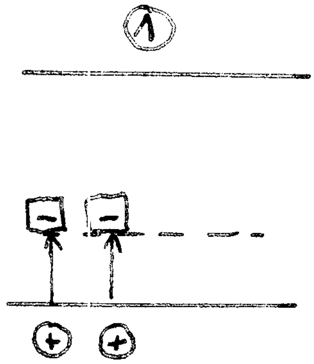
Assuming $v_H^{(e)} \propto v_H^{(h)} = v_H$ we have

$$R_H = \frac{v_H}{e} \cdot \frac{p\mu_h^2 - n\mu_e^2}{(n\mu_e + p\mu_h)^2}$$

$R_H = 0$ if $n\mu_e^2 = p\mu_h^2$

The mobility of electrons μ_e is typically much higher than the mobility of holes μ_h. if e.g. $\mu_e = 10\mu_h$, then in p-type semiconductor at low T the conductivity is due to holes only

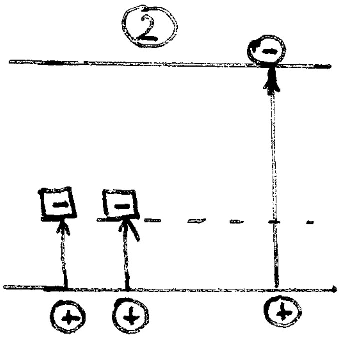
P-type



low T

holes

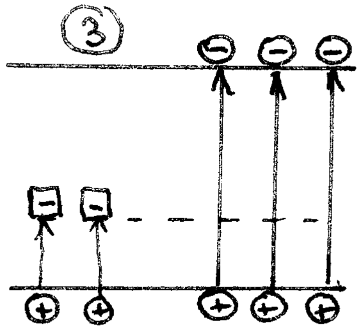
$R_H > 0$



higher T

holes + electrons

$R_H \approx 0$

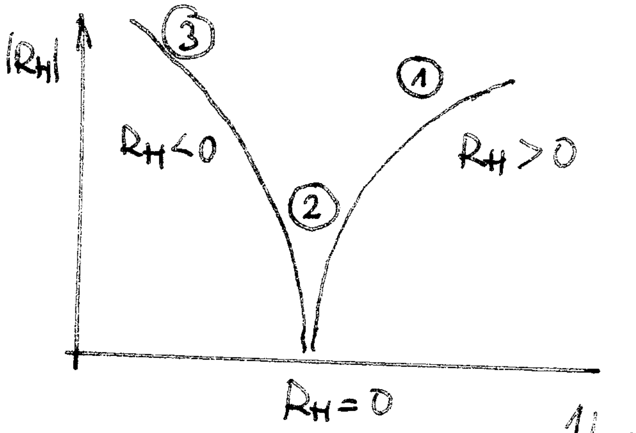


high T

$n \approx p$

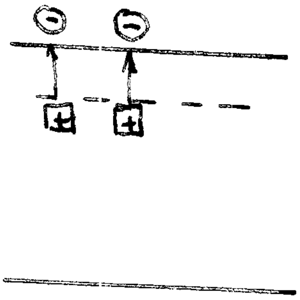
$R_H < 0$

due to $\mu_e > \mu_h$



$n\mu_e^2 = p\mu_h^2$

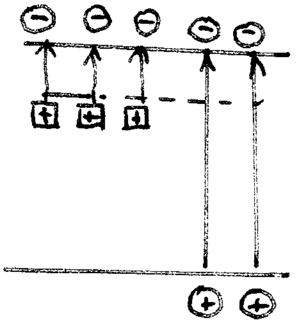
N-type



low T

electrons from donors

$R_H < 0$

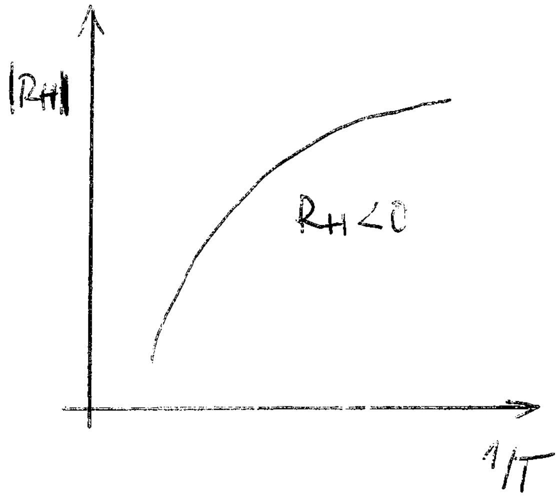


electrons + holes

but $n > p$

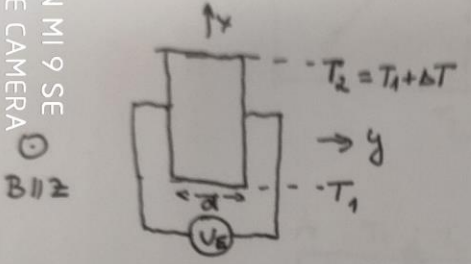
$\mu_e > \mu_h$

$R_H < 0$



Nernst- Ettingshausen effect

Formation of electric field in the direction „y" perpendicular to temperature gradient „x" and magnetic field B - „z"



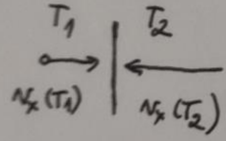
$$E_y = \frac{U_E}{d} = -Q B_z \nabla_x T =$$

$$= -Q B_z \Delta T$$

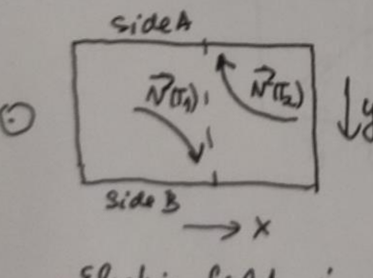
Q .. Nernst-Ettingshausen coefficient

Qualitative explanation

In every layer of the sample ⊥ to ∇T electrons move with thermal velocity in all directions



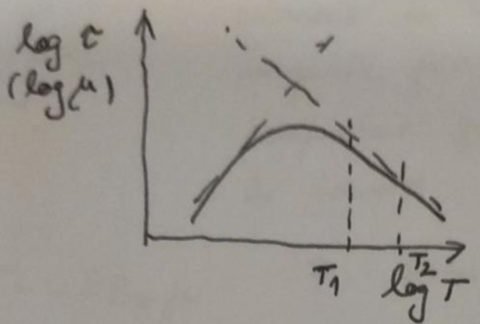
If on the lef hand side of the thought boundary the temperature is smaller, the $N_x(T_1)$ component is smaller than $N_x(T_2)$



The $\vec{v}(T_2)$ and $\vec{v}(T_1)$ electrons just close to the boundary are deflected to opposite sites in the magnetic field.

Electric field in the y direction is formed, if the streams of $\vec{v}(T_1)$ and $\vec{v}(T_2)$ electrons are different. The sign of the transversal voltage and electric field depend on the temperature dependence of the scattering mechanisms

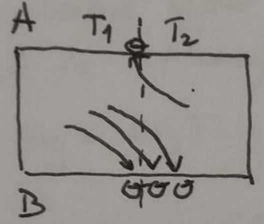
case I



In this case the $v(T_2)$ electrons scatter more than $v(T_1)$ electrons

$\mu(T_2) < \mu(T_1)$

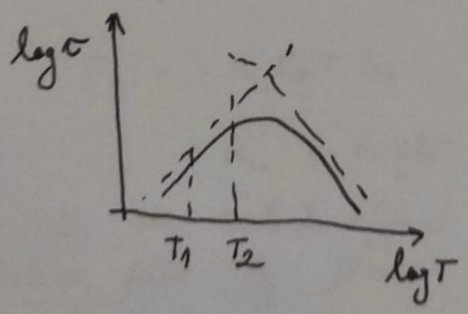
$\tau(T_2) < \tau(T_1)$



There are more electrons at side B than at side A

The direction of the E_y is ↓ A B

case II

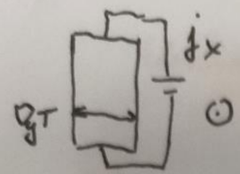


In this case the $v(T_2)$ electrons scatter less than $v(T_1)$ electrons.

The direction of E_y is ↑ A B

The sign of the effect is opposite

Ettingshausen effect



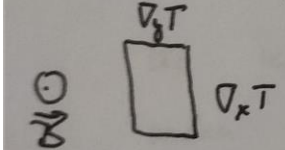
as a result of flow of electric current in the x direction when magnetic field B is in z direction, temperature gradient in y direction is formed

$\nabla_y T = -P B_z j_x$ P... Ettingshausen coefficient

Due to Seebeck effect this temperature gradient is transformed into electric field

$$E_y = \alpha \nabla_y T$$

Righi - Leduc effect



The temperature gradient in x direction in the magnetic field in z direction results in formation of temperature gradient in y direction.

$$\nabla_y T = - R_L \nabla_x T B_z$$

R_L... Righi - Leduc coefficient

Due to the Seebeck effect is then a transversal electric field E_y formed

$$E_y = \alpha \nabla_y T$$

Electrons and holes out of equilibrium

n_0, p_0 -- equilibrium concentrations

$\Delta n, \Delta p$ -- deviation from equilibrium

$\Delta n = n - n_0$ $\Delta p = p - p_0$ $\Delta n = \Delta p$

Let G_0 be a measure of the thermal generation of electron - hole pairs, which is always present

We will further examine the situation when after finishing of the excitation the system comes back to equilibrium.

We will use continuity equation for electrons

$$\frac{\partial n}{\partial t} = G - R + \frac{1}{e}\,\mathrm{div}\,\vec{j}_e = G - R - \mathrm{div}\,\vec{J}_e$$

G ... generation of electrons
R ... recombination of electrons
G_0 ... thermal generation of electrons

In equilibrium $G_0 = R_0$

Let as assume, that electrons are generated by emission from the valence band only (we will not include emission from donors in this case). Therefore also recombination occurs by interaction with holes from the valence band.

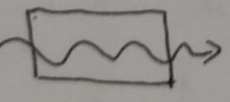
In equilibrium $G_0 = R_0 = r n_0 \cdot p_0$
r ... recombination coefficient

After switching-off the excitation $G = G_0$

$$\frac{\partial n}{\partial t} = G_0 - R + \frac{1}{e}\,\mathrm{div}\,\vec{j}_e$$

$R = r n p =$
$= r(n_0 + \Delta n)(p_0 + \Delta p)$

$\Delta n = \Delta p$
(generation and rec. over the bandgap)



Let us assume, that the sample is homogeneously illuminated which results in the deviation from equilibrium.

Due to homogeneous illumination $\operatorname{div} \vec{j}_e = 0$

$$\Rightarrow \quad -\frac{d\Delta n}{dt} = R - G_0 = r n p - r n_0 p_0 =$$

$$= r(n_0 + \Delta n)(p_0 + \Delta p) - r n_0 p_0 =$$

$$= r\left[n_0 p_0 + n_0 \Delta p + p_0 \Delta n + \Delta n \Delta p - n_0 p_0\right]$$

Let us suppose we have e.g. p-type semiconductor, i.e. $p_0 >> n_0$

$\Delta n = \Delta p$ (small – small deviation from equilibrium)

$\Rightarrow p_0 \Delta n >> n_0 \Delta p \qquad p_0 \Delta n >> \Delta n \Delta p$

$$\Rightarrow \quad -\frac{d\Delta n}{dt} = r p_0 \Delta n \qquad -\frac{d\Delta n}{\Delta n} = r p_0 dt$$

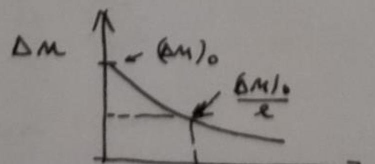
$$\frac{d\Delta n}{\Delta n} = -r p_0 dt = -\frac{dt}{\tau}$$

$$\Rightarrow \quad \ln \Delta n = -\frac{t}{\tau} + C$$

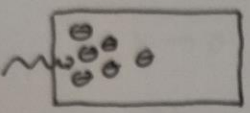
$t = 0 \quad \Delta n = (\Delta n)_0 \Rightarrow C = \ln (\Delta n)_0$

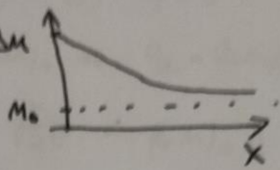
$$\Rightarrow (\Delta n)_t = (\Delta n)_0 \, e^{-\frac{t}{\tau}}$$

τ ... lifetime of minority electrons



In the next example we will examine stationary distribution of carriers when the sample is inhomogeneously illuminated





The continuity equation

$$\frac{\partial n}{\partial t} = G - R + \frac{1}{e}\,\mathrm{div}\,\vec{j_e} \qquad R = R_0 + R'$$

$$R_0 = G_0$$

$$\frac{\partial n}{\partial t} = r n_0 p_0 - r n_0 p_0 - R' + \frac{1}{e}\,\mathrm{div}\,\vec{j_e}$$

$$R' = r p_0 \Delta n = \frac{\Delta n}{\tau}$$ (for the case of p-type sc - previous case)

$$\Rightarrow \frac{\partial n}{\partial t} = -\frac{\Delta n}{\tau} + \frac{1}{e}\,\mathrm{div}\,\vec{j_e} \rightarrow \frac{\partial n}{\partial t} = -\frac{\Delta n}{\tau} + \frac{1}{e}\cdot\frac{\partial j_e}{\partial x}$$

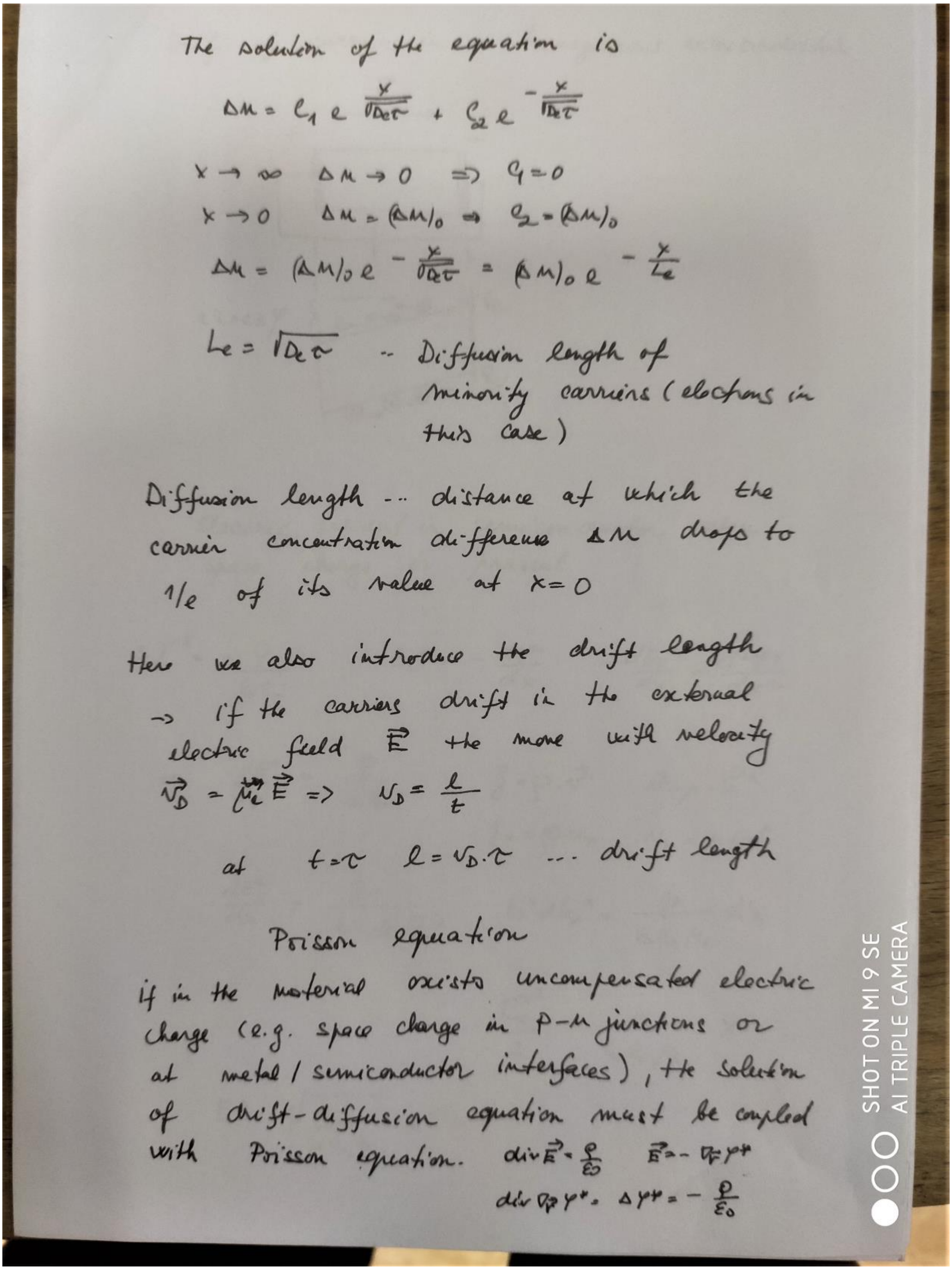
$\frac{\partial n}{\partial t} = 0$ in stationary case

$$\Rightarrow \frac{\Delta n}{\tau} = \frac{1}{e}\cdot\frac{\partial j_e}{\partial x} \qquad j_e = e D_e \cdot \frac{\partial n}{\partial x}$$

$$\Rightarrow \frac{\Delta n}{\tau} = D_e \cdot \frac{\partial^2 n}{\partial x^2}$$

(diffusion current) no drift current because there is no external el. field.

Diffusion equation



The solution of the equation is

$$\Delta n = C_1 e^{\frac{x}{\sqrt{D_e \tau}}} + C_2 e^{-\frac{x}{\sqrt{D_e \tau}}}$$

$x \to \infty \quad \Delta n \to 0 \quad \Rightarrow C_1 = 0$

$x \to 0 \quad \Delta n = (\Delta n)_0 \Rightarrow C_2 = (\Delta n)_0$

$$\Delta n = (\Delta n)_0 e^{-\frac{x}{\sqrt{D_e \tau}}} = (\Delta n)_0 e^{-\frac{x}{L_e}}$$

$L_e = \sqrt{D_e \tau}$ -- Diffusion length of minority carriers (electrons in this case)

Diffusion length ... distance at which the carrier concentration difference Δn drops to $1/e$ of its value at $x = 0$

Here we also introduce the drift length

→ if the carriers drift in the external electric field $\vec{E}$ the move with velocity

$\vec{v}_D = -\mu_e \vec{E} \Rightarrow v_D = \frac{l}{t}$

at $t = \tau \quad l = v_D \cdot \tau$ ... drift length

Poisson equation

if in the material exists uncompensated electric charge (e.g. space charge in p-n junctions or at metal / semiconductor interfaces), the solution of drift-diffusion equation must be coupled with Poisson equation. $\operatorname{div} \vec{E} = \frac{\rho}{\varepsilon_0} \quad \vec{E} = -\nabla_{\vec{r}} \varphi^*$

$$\operatorname{div} \nabla_{\vec{r}} \varphi^* = \Delta \varphi^* = -\frac{\rho}{\varepsilon_0}$$

The solution of the equation is

$$\Delta n = C_1 e^{\frac{x}{\sqrt{D_e \tau}}} + C_2 e^{-\frac{x}{\sqrt{D_e \tau}}}$$

$x \to \infty \quad \Delta n \to 0 \quad \Rightarrow C_1 = 0$

$x \to 0 \quad \Delta n = (\Delta n)_0 \Rightarrow C_2 = (\Delta n)_0$

$$\Delta n = (\Delta n)_0 e^{-\frac{x}{\sqrt{D_e \tau}}} = (\Delta n)_0 e^{-\frac{x}{L_e}}$$

$L_e = \sqrt{D_e \tau}$ .. Diffusion length of minority carriers (electrons in this case)

Diffusion length ... distance at which the carrier concentration difference Δn drops to $1/e$ of its value at $x = 0$

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at $t = \tau \quad l = v_D \cdot \tau$ ... drift length

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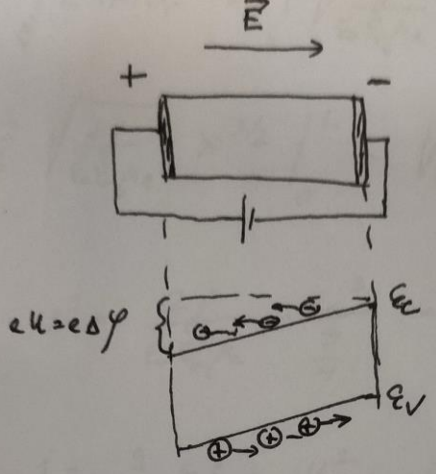
$\mathrm{div}\,\nabla_{\vec{r}} \varphi = \Delta \varphi = -\frac{\varrho}{\varepsilon_0}$

Drift of carriers in a homogeneous semiconductor



Electric current in semiconductor when space charge is present

$$\Delta\varphi^* = -\frac{\rho}{\varepsilon_0\varepsilon_r} \qquad E_x^* = -\frac{d\varphi^*}{dx} \qquad -\frac{dE_x^*}{dx} = \frac{d^2\varphi^*}{dx^2}$$

$$\Rightarrow \quad \frac{dE^*}{dx} = \frac{\rho}{\varepsilon_0\varepsilon_r} \qquad \vec{j} = \rho\cdot\vec{v} \qquad \vec{v} = \mu\cdot\vec{E}^*$$

$$j_x = \rho v_x \qquad v_x = \mu E_x^*$$

$$\frac{dE_x^*}{dx} = \frac{j_x}{\varepsilon_0\varepsilon_r\mu_x E_x^*} \qquad E_x^* dE_x^* = \frac{j_x}{\varepsilon_0\varepsilon_r\mu_{ex}}dx$$

$$\frac{E_x^{*2}}{2} = \frac{j_x}{\varepsilon_0\varepsilon_r\mu_e}\cdot x$$

$$E_x^* = \sqrt{\frac{2j}{\varepsilon_0\varepsilon_r\mu_x}}\ x^{1/2}$$

$$U = \int_0^L E^*(x)\,dx = \int_0^L \sqrt{\frac{2j}{\varepsilon_0 \varepsilon_r \mu_e}}\; x^{1/2}\,dx =$$

$$= \frac{2}{3}\sqrt{\frac{2j}{\varepsilon_0 \varepsilon_r \mu_e}}\; x^{3/2}\Big|_0^L = \sqrt{\frac{2j}{\varepsilon_0 \varepsilon_r \mu_e}} \cdot \frac{L^{3/2}}{\frac{3}{2}}$$

$$\Rightarrow \quad U^2 = \frac{2j}{\varepsilon_0 \varepsilon_r \mu_e} \cdot \frac{L^3}{\frac{9}{4}} = \frac{8}{9} \cdot \frac{j}{\varepsilon_0 \varepsilon_r \mu_e} L^3$$

$$j = \frac{9}{8}\varepsilon_0 \varepsilon_r \mu_e \frac{U^2}{L^3}$$ (Mott - Gurney law)

Electric current in vacuum

The potential energy of the electron $-e\varphi^*(x)$ changes into the kinetic energy of the accelerated electron

$$e\varphi^* = \frac{1}{2} m v^2 \qquad \frac{dE^*}{dx} = \frac{\rho}{\varepsilon_0 \varepsilon_r} \qquad E^* = -\frac{d\varphi^*}{dx}$$

$$v = \sqrt{\frac{2e\varphi^*}{m_e}} \qquad \rho = \frac{j}{v} = j \cdot \sqrt{\frac{m}{2e\varphi^*}} \qquad \frac{d^2\varphi^*}{dx^2} = \frac{\rho}{\varepsilon_0 \varepsilon_r}$$

$$\frac{dE^*}{dx} = \frac{dE^*}{d\varphi^*} \cdot \frac{d\overset{1-E}{\varphi^*}}{dx} = \frac{\rho}{\varepsilon_0} = \frac{j}{\varepsilon_0}\sqrt{\frac{m}{2e\varphi}}$$

$$E^* = -\frac{d\varphi^*}{dx}$$

$$-E^* dE^* = \frac{dE^*}{dx} d\varphi^* = \frac{j}{\varepsilon_0} \cdot \sqrt{\frac{m}{2e\varphi}}\, d\varphi^*$$

$$-\frac{E^{*2}}{2} = \frac{j}{\varepsilon_0} \cdot 2\sqrt{\frac{m}{2e}} \cdot \varphi^{*1/2}$$

$$E^{*2} = -\frac{j}{\varepsilon_0} 4\sqrt{\frac{m}{2e\varphi^*}}$$

$$E^* = -2\sqrt{\frac{j}{\varepsilon_0}\sqrt{\frac{m}{2e\varphi^*}}} = -2\sqrt{\frac{j}{\varepsilon_0}\sqrt{\frac{m}{2e}}}\ \varphi^{*1/4}$$

$$E^* = -\alpha\varphi^{*1/4} \qquad \alpha = 2\sqrt{\frac{j}{\varepsilon_0}\sqrt{\frac{m}{2e}}}$$

$$E^* = -\frac{d\varphi^*}{dx} = -\alpha\varphi^{*1/4}$$

$$\alpha\, dx = \varphi^{*-1/4} d\varphi$$

$$\alpha x\Big|_0^L = \frac{4}{3}\varphi^{*3/4}$$

$$\alpha L = \frac{4}{3}\varphi^{*3/4} \qquad \varphi^* \Rightarrow u$$

$$\alpha L = \frac{4}{3}u^{3/4} \qquad \alpha^2 L^2 = \frac{16}{9}u^{3/2}$$

$$4\frac{j}{\varepsilon_0}\sqrt{\frac{m}{2e}}\, L^2 = \frac{16}{9}u^{3/2}$$

$$j = \frac{4}{9} \cdot \varepsilon_0 \cdot \sqrt{\frac{2e}{m}} \cdot \frac{u^{3/2}}{L^2}$$

Ambipolar mobility and diffusion constant

When describing the deviation from equilibrium we assumed so far, that the semiconductor is a clear n-type or p-type. Then it is possible to include only excess minority electrons in p-type (Δn) or excess holes in N-type (Δp). In case, that both Δn and Δp are present (i.e. $\Delta n \gg p_0$ and at the same time $\Delta p \gg n_0$); Δn and Δp can mutually influence – the transport is in this situation described as „ambipolar"

$$\vec{j}_e = e n \mu_e \vec{E} + e D_e \nabla_{\vec{r}} n$$
$$\vec{j}_h = e p \mu_h \vec{E} - e D_h \nabla_{\vec{r}} p$$

Drift-diffusion equation

$$\frac{\partial n}{\partial t} = G - R + \frac{1}{e} \operatorname{div} \vec{j}_e$$

Continuity equation

$$\frac{\partial p}{\partial t} = G - R - \frac{1}{e} \operatorname{div} \vec{j}_h$$

$$\frac{\partial n}{\partial t} = G - R + \mu_e \operatorname{div}(n\vec{E}) + \cancel{e} D_e \operatorname{div} \nabla_{\vec{r}} n$$

$$\frac{\partial p}{\partial t} = G - R - \mu_h \operatorname{div}(p\vec{E}) + D_h \operatorname{div} \nabla_{\vec{r}} p$$

$n = n_0 + \Delta n \qquad p = p_0 + \Delta p \qquad \Delta n = \Delta p$

$$\frac{\partial n_0}{\partial t} = \frac{\partial p_0}{\partial t} = 0 \qquad \mathrm{grad}_{\vec r}\, n_0 = \mathrm{grad}_{\vec r}\, p_0 = 0$$

$$\frac{\partial n}{\partial t} = G - R + \mu_e \vec E\, \mathrm{grad}_{\vec r}(\Delta n) + \mu_e n\, \mathrm{div}\, \vec E + D_e \overset{\text{operator}}{\Delta}(\Delta n)$$

$$\frac{\partial p}{\partial t} = G - R - \mu_h \vec E\, \mathrm{grad}_{\vec r}(\Delta p) - \mu_h p\, \mathrm{div}\, \vec E + D_h \Delta(\Delta p)$$

$$\mathrm{div}\, \vec E = \frac{1}{\mu_e n}\left(\frac{\partial \Delta n}{\partial t} - G + R + \mu_e \vec E\, \mathrm{grad}_{\vec r}(\Delta n)\right) + D_e \Delta(\Delta n) \quad (1)$$

$$\mathrm{div}\, \vec E = -\frac{1}{\mu_h p}\left(\frac{\partial \Delta n}{\partial t} - G + R + \mu_h \vec E\, \mathrm{grad}_{\vec r}(\Delta n) - D_h \Delta(\Delta n)\right) \quad (2)$$

(1) − (2)

$$0 = \frac{\partial \Delta n}{\partial t}\left(\frac{1}{n\mu_e} + \frac{1}{p\mu_h}\right) + (R-G)\left(\frac{1}{n\mu_e} + \frac{1}{p\mu_h}\right) - \frac{1}{n}\vec E\, \mathrm{grad}_{\vec r}(\Delta n) +$$

$$+ \frac{1}{p}\left(\vec E \cdot \mathrm{grad}_{\vec r}(\Delta p)\right) - \frac{D_e}{n\mu_e}\Delta(\Delta n) - \frac{D_p}{p\mu_h}\Delta(\Delta n)$$

$$\frac{\partial \Delta n}{\partial t} = \frac{1}{\left(\frac{1}{n\mu_e} + \frac{1}{p\mu_p}\right)}\left[(G-R)\left(\frac{1}{n\mu_e} + \frac{1}{p\mu_h}\right) + \left(\frac{1}{n} - \frac{1}{p}\right)\vec E\, \mathrm{grad}_{\vec r}(\Delta n) + \right.$$

$$\left. + \frac{D_e}{n\mu_e}\Delta(\Delta n) + \frac{D_h}{p\mu_h}\Delta(\Delta n)\right]$$

$$\frac{\partial \Delta n}{\partial t} = G - R + \frac{(p-n)\mu_e\mu_h}{n\mu_h + p\mu_h}\vec E \cdot \mathrm{grad}_{\vec r}(\Delta n) +$$

$$+ \frac{D_e p\mu_h + D_h n\mu_n}{n\mu_e + p\mu_h}\Delta(\Delta n)$$

$$\frac{\partial \Delta n}{\partial t} = G - R + \mu^* \vec{E}\, \mathrm{grad}_{\vec{r}}(\Delta n) + D^* \Delta(\Delta n)$$

Laplace operator

$$\mu^* = \frac{(p-n)\mu_e \mu_h}{n\mu_e + p\mu_h} = \frac{p-n}{\frac{p}{\mu_e} + \frac{n}{\mu_h}}$$

ambipolar mobility

$$D^* = \frac{p+n}{\frac{p}{D_e} + \frac{n}{D_h}}$$ ambipolar diffusion constant

For $p = n$ $\mu^* = 0$

(a group of excess carriers $\Delta n = \Delta p$ does not move in an electric field – only diffusion takes place ⇒ the shape of the group packet is changing.)

strong N-type $\mu^* = \frac{-n}{\frac{n}{\mu_h}} = -\mu_h$ $D^* = D_h$

strong P-type $\mu^* = \mu_e$ $D^* = D_e$

Ambipolar mobility and diffusion constant

When describing the deviation from equilibrium we assumed so far, that a semiconductor is a clear N-type or clear p-type. Then it is possible to study only excess minority carriers (Δn in p-type, Δp in n-type). The excess of majority carriers is in this case negligible compared to their equilibrium values ($\Delta n \ll n_0$ in n-type, $\Delta p \ll p_0$ in p-type). In case, that the excess values $\Delta n / \Delta p$ are higher or if $\Delta n \lesssim n_0$ in n-type or $\Delta p \lesssim p_0$ in p-type), we have to include both excesses $\Delta n, \Delta p$ in the calculation and take into account, that both charge clouds influence each other. The transport is in this situation described as ambipolar.

$$\vec{j}_e = e n \mu_e \vec{E} + e D_e \nabla_{\vec{r}} n$$
$$j_h = e p \mu_h \vec{E} - e D_h \nabla_{\vec{r}} p$$

Drift-diffusion equation

$$\frac{\partial n}{\partial t} = G - R + \frac{1}{e} \operatorname{div} \vec{j}_e$$
$$\frac{\partial p}{\partial t} = G - R - \frac{1}{e} \operatorname{div} \vec{j}_h$$

Continuity equation

$$\frac{\partial n}{\partial t} = G - R + \mu_e \cancel{e} \operatorname{div}(n\vec{E}) + D_e \operatorname{div} \nabla_{\vec{r}} n$$
$$\frac{\partial p}{\partial t} = G - R - \mu_h \operatorname{div}(p\vec{E}) + D_h \operatorname{div} \nabla_{\vec{r}} p$$

$$n = n_0 + \delta n \qquad p = p_0 + \delta p \qquad \delta n = \delta p$$

$$\frac{\partial n_0}{\partial t} = \frac{\partial p_0}{\partial t} = 0 \qquad \mathrm{grad}_{\vec{r}}\, n_0 = \mathrm{grad}_{\vec{r}}\, p_0 = 0$$

(homogeneous semiconductor)

$$\frac{\partial n}{\partial t} = G - R + \mu_e \vec{E}\, \mathrm{grad}_{\vec{r}}\, (\delta n) + \mu_e n\, \mathrm{div}\, \vec{E} + D_e \overset{\swarrow \mathrm{div}\, \mathrm{grad}_{\vec{r}}}{\Delta} (\delta n)$$

$$\frac{\partial p}{\partial t} = G - R - \mu_h \vec{E}\, \mathrm{grad}_{\vec{r}}\, (\delta p) - \mu_h p\, \mathrm{div}\, \vec{E} + D_h \Delta (\delta p)$$

$$\mathrm{div}\, \vec{E} = \frac{1}{\mu_e n} \left(\frac{\partial \delta n}{\partial t} - G + R + \mu_e \vec{E}\, \mathrm{grad}_{\vec{r}}\, \delta n) + D_e \Delta (\delta n) \right) \quad (1)$$

$$\mathrm{div}\, \vec{E} = -\frac{1}{\mu_h p} \left(\frac{\partial \delta n}{\partial t} - G + \overset{\delta n = \delta p}{\overset{\downarrow}{R}} + \mu_h \vec{E}\, \mathrm{grad}_{\vec{r}}\, \delta n - D_h \Delta (\delta n) \right) \quad (2)$$

$(1) - (2) \Rightarrow$

$$0 = \frac{\partial \delta n}{\partial t} \left(\frac{1}{n\mu_e} + \frac{1}{p\mu_h} \right) + (R - G) \left(\frac{1}{n\mu_e} + \frac{1}{p\mu_h} \right) - \frac{1}{n} \vec{E}\, \mathrm{grad}_{\vec{r}} (\delta n) +$$

$$+ \frac{1}{p} (\vec{E} \cdot \nabla_{\vec{r}} (\delta n) - \frac{D_e}{n\mu_e} \Delta (\delta n) - \frac{D_h}{p\mu_h} \Delta (\delta n))$$

$$\frac{\partial \delta n}{\partial t} = \frac{1}{\left(\frac{1}{n\mu_e} + \frac{1}{p\mu_h} \right)} \left[G - R \left(\frac{1}{n\mu_e} + \frac{1}{p\mu_h} \right) + \left(\frac{1}{n} - \frac{1}{p} \right) \vec{E}\, \mathrm{grad}_{\vec{r}} (\delta n) + \right.$$

$$\left. + \frac{D_e}{n\mu_e} \Delta (\delta n) + \frac{D_h}{p\mu_h} \Delta (\delta n) \right]$$

$$\frac{\partial \delta n}{\partial t} = G - R + \frac{(p - n) \mu_e \mu_h}{n\mu_e + p\mu_h} \vec{E} \cdot \nabla_{\vec{r}} (\delta n) +$$

$$+ \frac{D_e p \mu_h + D_h n \mu_e}{n\mu_e + p\mu_h} \Delta (\delta n)$$

$$\frac{\partial \Delta n}{\partial t} = G - R + \mu^* \vec{E}\, \mathrm{grad}_{\vec{r}}(\Delta n) + D^* \overset{\text{Laplace}}{\Delta} (\Delta n)$$

$$\mu^* = \frac{(p-n)\mu_e \mu_h}{n\mu_e + p\mu_h} = \frac{p-n}{\frac{p}{\mu_e} + \frac{n}{\mu_h}}$$

↑

ambipolar mobility

$$D^* = \frac{p+n}{\frac{p}{D_e} + \frac{n}{D_h}}$$ ambipolar diffusion constant

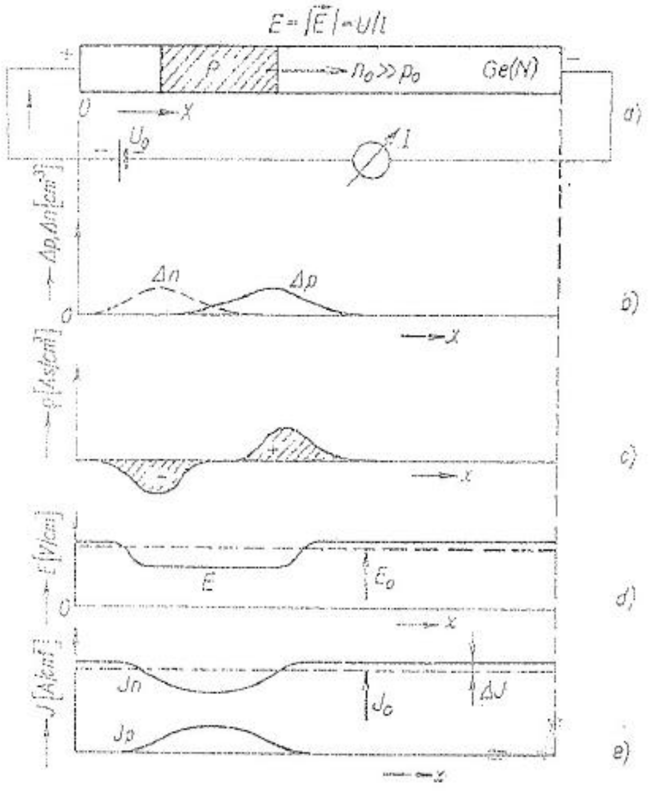
For $p = n$ $\quad \mu^* = 0$

(group of excess carriers $\Delta n = \Delta p$ does not move in an electric field; only diffusion takes place; the shape of the group packet is changing

Strong N-type $\quad \mu^* = -\frac{n}{\frac{n}{\mu_h}} = -\mu_h \quad D^* = D_h$

Strong P-type $\quad \mu^* = \mu_e \quad D^* = D_e$

Movement of injected group of minority carriers



a) Sample with the applied voltage

b) local distribution of excess carriers

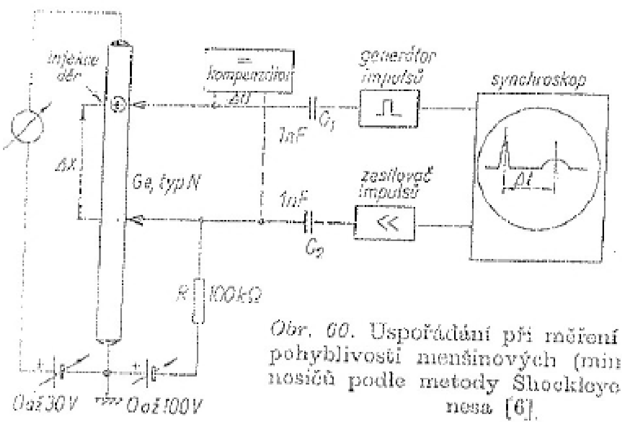
c) distribution of space charge

d) profile of electric field

e) density of flow of electrons and holes

In the electric field the groups of excess electrons and holes spatially separate. Then an additional electric field between them is formed against the direction of the external field E_0. The electric field between Δn and Δp is smaller than E_0, outside it is slightly higher. The average internal field must equal E_0.

Shockley - Haynes experiment



Obr. 60. Uspořádání při měření driftové pohyblivosti menšinových (minoritních) nosičů podle metody Shockleye a Haynesa [6].

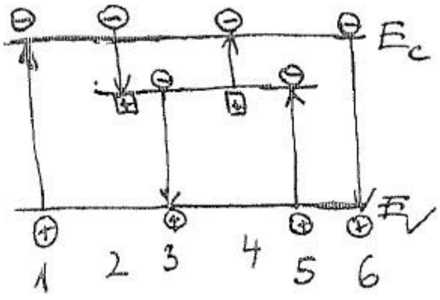
$$\overline{v} = \mu^* |E_0| = \frac{\Delta x}{t} = \mu^* \frac{\Delta U}{\Delta x}$$

$$\Rightarrow \mu^* = \frac{(\Delta x)^2}{\Delta U \cdot t}$$

Influence of trapping and recombination centers on charge transport

When deriving equations for diffusion length and lifetime of minority carriers we assumed so far, that free electrons in conduction band recombine with free holes in the valance band. Therefore, we did not account for influence of energy levels in the bandgap.

The influence of energy levels on transport of charge can be described by the so called Shokley-Read-Hall model.

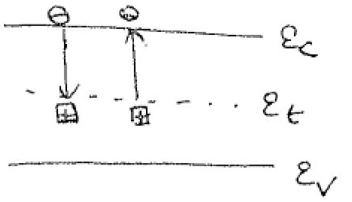


Each energy level can interact with the carriers in conduction and valence bands by a series of processes. all processes including interband are:

1) Interband generation
2) Trapping of electrons on level
3) Trapping of hole on the level
4) Emission of electron from the level
5) Emission of hole from the level
6) Interband recombination

Each level can be characterized by the following parameters

σ_e ..	capture-cross section for electrons	$[cm^2]$
σ_h	capture-cross section for holes	$[cm^2]$
ε_t	energy of the level	$[eV]$
N_t	concentration of the level	$[cm^{-3}]$
n_t	concentration of electrons on the level (occupied states)	$[cm^{-3}]$
$N_t - n_t$	concentration of unoccupied states on the level	$[cm^{-3}]$
γ_e	.. trapping coefficient for electrons ($\gamma_e = \sigma_e \cdot v_{th}^e$) v_{th}^e .. thermal velocity e	$[\frac{cm^3}{s}]$
γ_h	trapping coefficient for holes ($\gamma_h = \sigma_h \cdot v_{th}^h$) v_{th}^h .. thermal velocity, holes	$[cm^3/s]$



Trapping of electrons on the level

$$\frac{dn}{dt} = \gamma_e \cdot n\,(N_t - n_t)$$

in equilibrium
$n = n_0$
$n_t = n_{t0}$

Emission of electrons

$$\frac{dn_t}{dt} = \alpha\, n_t$$

α ... some coefficient we will try to calculate

Let us suppose that there is thermodynamic equilibrium

n_0 .. equilibrium concentration of electrons in the conduction band

n_{t0} equilibrium concentration of electrons on the level

$$\frac{dn_0}{dt} = \underbrace{\alpha_e \cdot n_{t0}}_{\uparrow} - \gamma_e \underbrace{n_0 (N_t - n_{t0})}_{\uparrow}$$

Probability of emission of electron from the center to the conduction band

Probability of trapping of an electron on the level in the bandgap

$\frac{dn_0}{dt} = 0$ in equilibrium

$$\Rightarrow \quad n_{t0} = \frac{N_t}{\frac{\alpha_e}{\gamma_e n_0} + 1}$$

at the same time $n_{t0} = N_t \cdot f_0$

$$f_0 = \frac{1}{1 + e^{\frac{\varepsilon - \varepsilon_F}{kT}}} = \frac{1}{1 + e^{x - \eta}}$$

$$n_0 \approx N_c e^{\eta} = N_c e^{\frac{\varepsilon_F}{kT}}$$

$$\Rightarrow \quad \frac{\alpha_e}{\gamma_e n_0} = e^{\frac{E_t - E_F}{kT}} \qquad (E = E_t \text{ in our case})$$

$$\Rightarrow \quad \alpha_e = \gamma_e n_0 e^{\frac{E_t - E_F}{kT}} \qquad N_c = n_0 e^{-\frac{E_F}{kT}}$$

$$\Rightarrow \alpha_e = \gamma_e N_c e^{\frac{E_t}{kT}} \quad ; \quad \alpha_e = \gamma_e \cdot n_1$$

$n_1 = N_c e^{\frac{E_t}{kT}}$ ... concentration of electrons for the case $E_t = E_F$

By a similar way we achieve

$$\alpha_h = \gamma_h \cdot p_1$$

p_1 .. concentration of holes for the case $E_t = E_F$

$N_t - n_t$ ... concentration of trapped holes

$$\frac{dn}{dt} = G + \underset{\substack{\uparrow \\ \text{electrons emitted} \\ \text{from the level} \\ \text{to the CB}}}{\gamma_e \cdot n_t \cdot n_1} - \underset{\substack{\uparrow \\ \text{Electrons trapped} \\ \text{on the level -} \\ \text{- transition from} \\ \text{CB to the level}}}{\gamma_e n (N_t - n_t)}$$

$$\frac{dp}{dt} = G + \underset{\uparrow}{\overset{\textcircled{5}}{\gamma_h (N_t - n_t) \cdot p_1}} - \underset{\nwarrow}{\overset{\textcircled{3}}{\gamma_h\, p \cdot n_t}}$$

transition of electron
from valence band
to the level (free hole
generation)

Transition of
electron from the
level to the valence
band = trapping
of hole

$$\frac{dn_t}{dt} = \gamma_e n (N_t - n_t) - \gamma_e n_t n_1 + \gamma_h (N_t - n_t) p_1 - \gamma_h p \cdot n_t$$

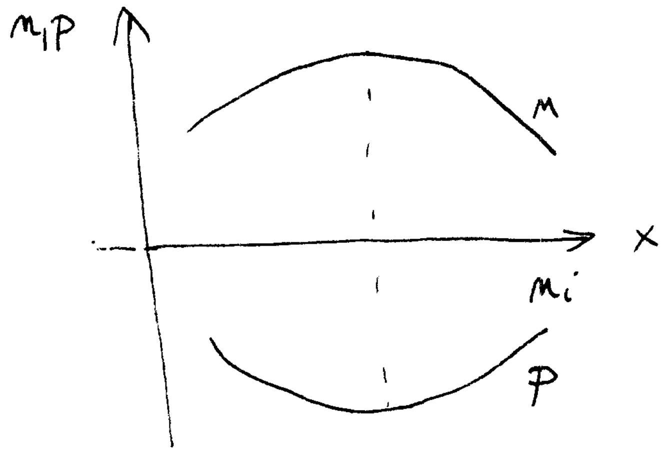
$\sigma_e = \sigma_h$ ... recombination center

$\sigma_e > \sigma_h$ ... electron trap

$\sigma_e < \sigma_h$ ... hole trap

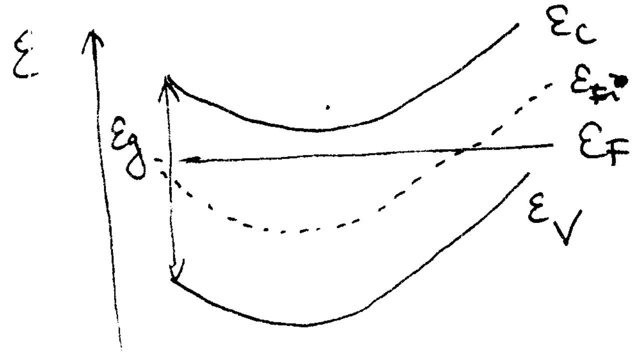
Inhomogeneous semiconductors

In the next part we will discuss theoretical description of inhomogeneous semiconductors, where the inhomogeneity is caused by change of doping in the SC volume, that results in variation of concentration of free electrons and holes with a spatial coordinate



We assume an N-type semiconductor here

$$n \cdot p = n_i^2$$



$\mathcal{E}_{Fi}$ ... intrinsic Fermi level defined by equation

$$n_i = N_c e^{\frac{\mathcal{E}_{Fi}}{kT}}$$

n_i .. intrinsic concentration

In equilibrium is the Fermi level $\mathcal{E}_F$ independent of x. The spatial variation of n and p is reflected in spatial dependence of the bands $\mathcal{E}_C(x)$, $\mathcal{E}_V(x)$ and also $\mathcal{E}_{Fi}(x)$. We introduce the difference $\mathcal{E}_F - \mathcal{E}_{Fi}(x)$ as the measure of spatial inhomogeneity.

We can write

$$n(x) = N_c e^{\frac{\varepsilon_F}{kT}} \qquad n_i = N_c e^{\frac{\varepsilon_{Fi}}{kT}} \Rightarrow N_c = n_i e^{-\frac{\varepsilon_{Fi}}{kT}}$$

then $$n = n_i e^{\frac{\varepsilon_F - \varepsilon_{Fi}}{kT}} \qquad \ln \frac{n}{n_i} = \ln \bar{n} = \frac{\varepsilon_F - \varepsilon_{Fi}(x)}{kT} =$$

$$= \psi = \frac{eV}{kT}$$

$$\Rightarrow \quad V = \frac{kT}{e} \cdot \psi$$ ψ is the so called reduced potential

$$np = n_i^2 \quad \Rightarrow \quad \frac{n}{n_i} = \frac{n_i}{p} \quad ; \quad \ln \frac{n}{n_i} = -\ln \frac{p}{n_i} = -\ln \bar{p}$$

The potential V caused by the spatial profile of the energy bands results in formation of internal electric field

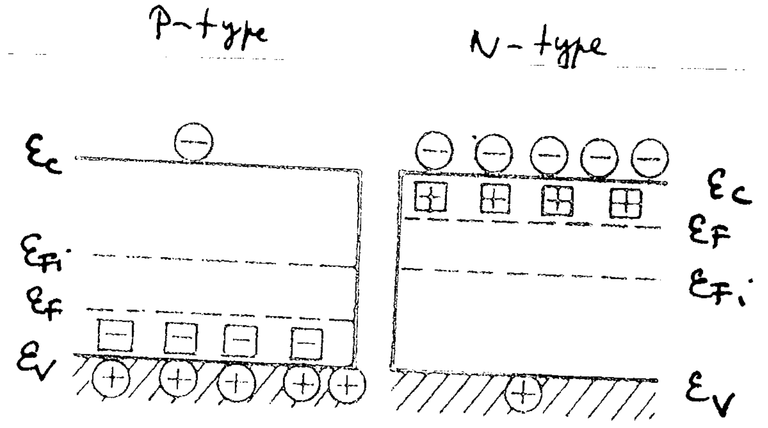
$$E^* = -\nabla_{\vec{r}} V = -\frac{kT}{e} \nabla_{\vec{r}} \psi = -\frac{kT}{e} \nabla_{\vec{r}} \ln \bar{n} =$$

$$= -\frac{kT}{e} \cdot \frac{\nabla_{\vec{r}} \bar{n}}{\bar{n}} = \frac{kT}{e} \frac{\nabla_{\vec{r}} \bar{p}}{\bar{p}}$$

Therefore in any inhomogeneous semiconductor exists an internal electric field. There is no net electric current, because the drift current due to the E-field is compensated in equilibrium with diffusion current caused by the gradient of concentration of corresponding carriers (electrons or holes).

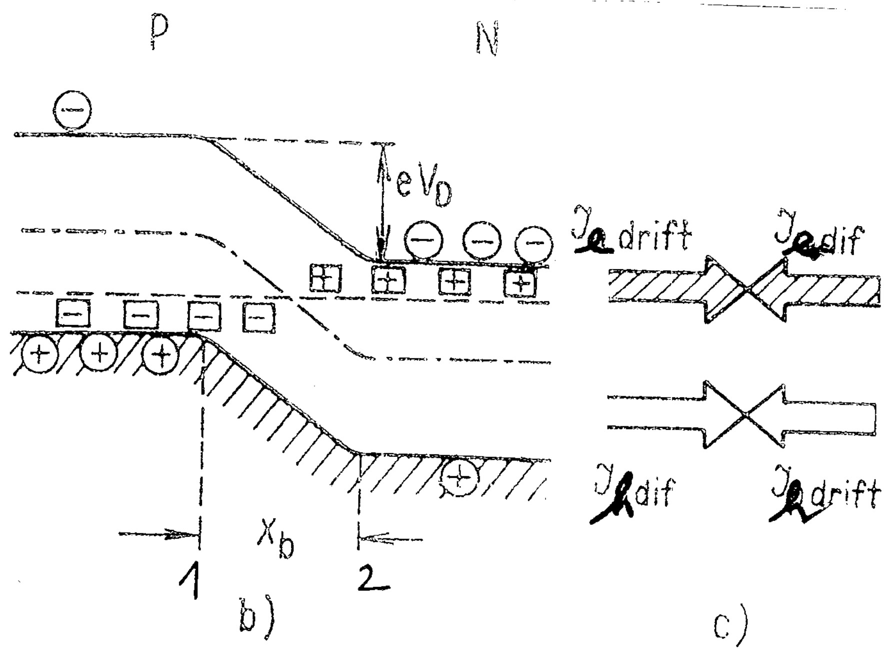
P-N junction

The P-N junction is a transition region between two parts of the same semiconductor, part of which is doped by acceptors, part by donors.



Semiconducta before P-N juction formation

The Fermi energy in P-type is lower than in N-type. After formion of P-N junction the Fermi energy must be everywhere the same.



Semiconductor after formation of P-N junction.

X_b ... width of the space charge region

During the formation of the P-N junction

1) Electrons from n-type diffuse to p-type due to the $\nabla_{\vec{r}} n$
2) Holes from p-type diffuse to n-type due to $\nabla_{\vec{r}} p$
3) As a result of diffusion of electrons from n-type, uncompensated positively charged donor atoms form a region of $\boxed{+}$ charge in N-type. By the same mechanism, negative space charge of uncompensated acceptors is created in P-type
4) Space charge distribution results in creation of an internal electric field This E-field opposes the diffusion currents
5) As a result of constant E_F throughout the material, an energy step eV_D is created in the energy diagram. Here V_D is the so called diffusion potential

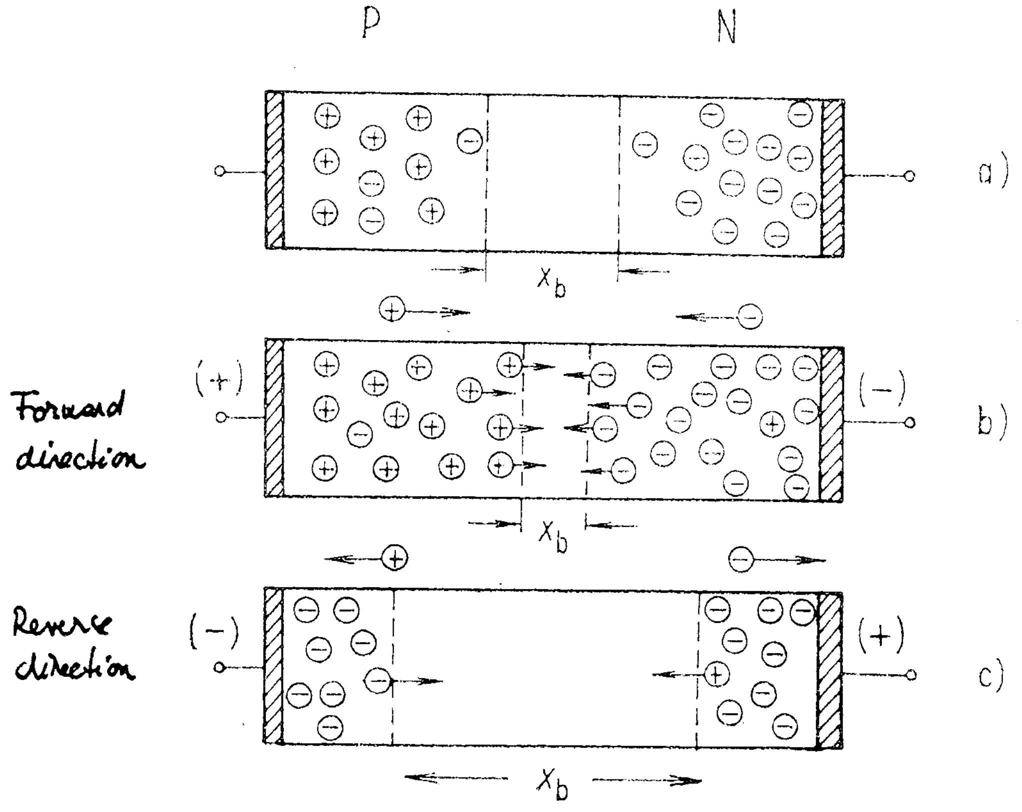
$$V_D = V_2 - V_1 = \frac{kT}{e}\left(\ln \bar{n}_2 - \ln \bar{n}_1\right) = \frac{kT}{e} \ln \frac{n_{n0}}{n_{p0}}$$

n_{n0} = Concentration of electrons in N-type in equilibrium (position 2)

n_{p0} = concentration of electrons in P-type in equilibrium (position 1)

P-N junction under bias

1) Forward direction (+) on P-type, (−) on N-type
Electrons from N-type are attracted to P-type. Holes from P-type are attracted to N-type. The space charge region is flooded by free carriers, the fixed charge of impurities is partially compensated, the width of the space charge region decreases. The injected minority carriers diffuse from the edge of the space charge region to the bulk. This diffusion results in the electric current, which is high.



The width of the space charge region without bias (a), in forward direction (b) and in reverse direction (c)

For the further calculation we set (1) at $x = 0$ and (2) at $x = x_b$

The excess of minority holes Δp_2 continues to move from (2) to the volume of the N-type by diffusion (there is nearly no electric field outside the space charge region, because the resistivity of this part is much higher than the resistivities of the neutral P and N-types and due to the Ohm law $U = (R_p + R_{sc} + R_n) I \approx$ $\approx R_{sc} I$ $(R_p I \ll R_{sc} I)$. According to the orientation of the x-axe the diffusion of holes takes place in the (+X) direction.

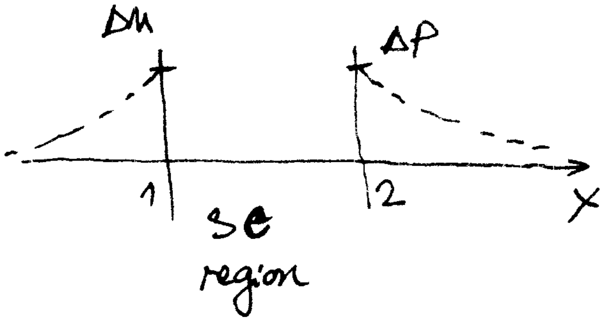
The excess of minority electrons Δn_1 diffuses to the P-type in (−x) direction.

From the example of return to equilibrium we were calculating, we know, that

$$\Delta p = \Delta p_2 \, e^{-\frac{(x - x_b)}{L_h}}$$

$$\Delta n = \Delta n_1 \, e^{\frac{x}{L_e}}$$

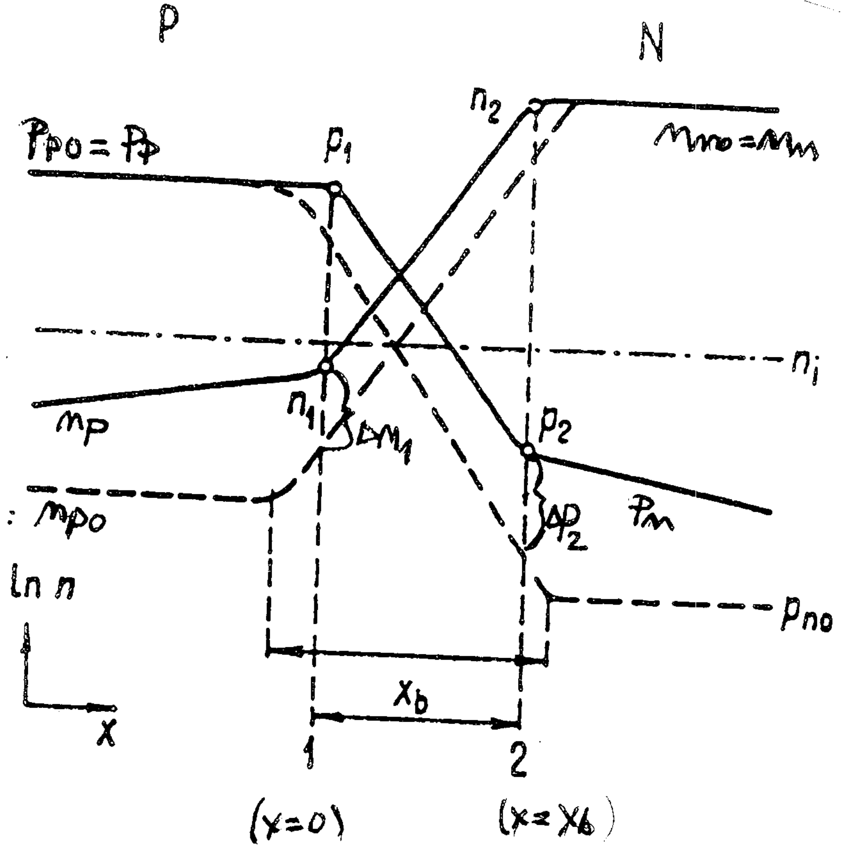
L_e, L_h diffusion lengths of electrons and holes



2) Reverse direction · (−) on P, (+) on N

The majority carriers are attracted from the edge of the space charge region to the contacts. The width of the space charge region increases compared to the situation without bias. Only minority carriers drift through the P−N junction (electrons from P-type are attracted by (+) on N and vice versa. The electric current in the reverse direction is composed of minority carriers and is small.

Calculation of the I-V characteristics



Here points (1) and (2) represent the edges of the space charge region under bias. In the picture we can see the forward direction.

We will calculate the contribution of excess carriers Δn_1 / Δp_2 to the electric current

$$j_e = e D_e \cdot \frac{d\Delta n}{dx} \qquad j_h = - e D_h \cdot \frac{d\Delta p}{dx}$$

$$\underbrace{\qquad\qquad}$$

diffusion terms of the drift-diffusion equation

$$j_e = e \cdot \frac{D_e}{L_e} \cdot \Delta n \qquad j_h = e \frac{D_h}{L_h} \cdot \Delta p$$

$$j = j_e + j_h$$

$$j = e \frac{D_e}{L_e} \cdot \Delta n_1 e^{\frac{x}{L_e}} \bigg|_{x=0} + e \frac{D_h}{L_h} \cdot \Delta p_2 e^{-\frac{(x-x_b)}{L_h}} \bigg|_{x=x_b}$$

$$j = e \frac{D_e}{L_e} \Delta n_1 + e \frac{D_h}{L_h} \cdot \Delta p_2$$

To calculate j we have to calculate Δn_1 and Δp_2 first

Equilibrium (no external voltage)

The diffusion potential

$$V_D = \frac{kT}{e} \ln \frac{n_{n0}}{n_{p0}} = -\frac{kT}{e} \ln \frac{p_{n0}}{p_{p0}} = \frac{kT}{e} \cdot \ln \frac{p_{p0}}{p_{n0}}$$

$$\Rightarrow \quad \frac{p_{n0}}{p_{p0}} = e^{-\frac{eV_D}{kT}}$$

after application of external voltage U'

$$V_D - U' = \frac{kT}{e} \ln \frac{p_1}{p_2}$$ (U' can be both positive and negative)

$$\frac{p_1}{p_2} = e^{\frac{e(V_D - u')}{kT}}$$

$$\frac{p_2}{p_1} = e^{-\frac{e(V_D - u')}{kT}} = \frac{p_{n0} + \Delta p_2}{p_{p0} + \Delta p_1}$$

$$e^{-\frac{V_D}{kT}} e^{\frac{eu'}{kT}} \approx \frac{p_{n0} + \Delta p_2}{p_{p0}} \qquad \Delta p_1 \ll p_{p0}$$

$$\frac{p_{n0}}{p_{p0}} e^{eu'/kT} = \frac{p_{n0} + \Delta p_2}{p_{p0}}$$

$$p_{n0} + \Delta p_2 = p_{n0} e^{\frac{eu'}{kT}}$$

$$\Delta p_2 = p_{n0} \left(e^{\frac{eu'}{kT}} - 1 \right)$$

In a similar way we can derive

$$\Delta n_1 = n_{p0} \left(e^{\frac{eu'}{kT}} - 1 \right)$$

Then

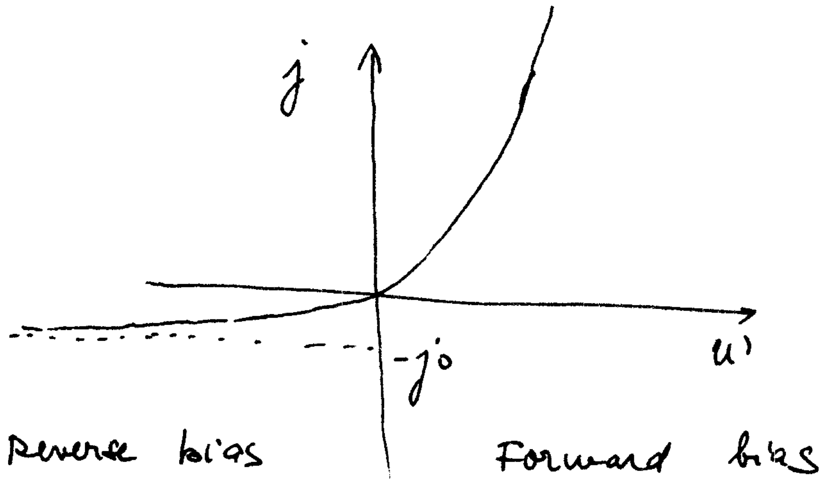
$$j = \left[e \frac{D_e}{L_e} \cdot n_{p0} + e \frac{D_h}{L_e} p_{n0} \right] \left(e^{\frac{eu'}{kT}} - 1 \right)$$

$$j = j_0 \left(e^{\frac{eu'}{kT}} - 1 \right)$$

For large $u' < 0$ $\quad e^{\frac{eu'}{kT}} \to 0$

and $j = -j_0$

(reverse current)


j
u
$-j_0$
Reverse bias
Forward bias

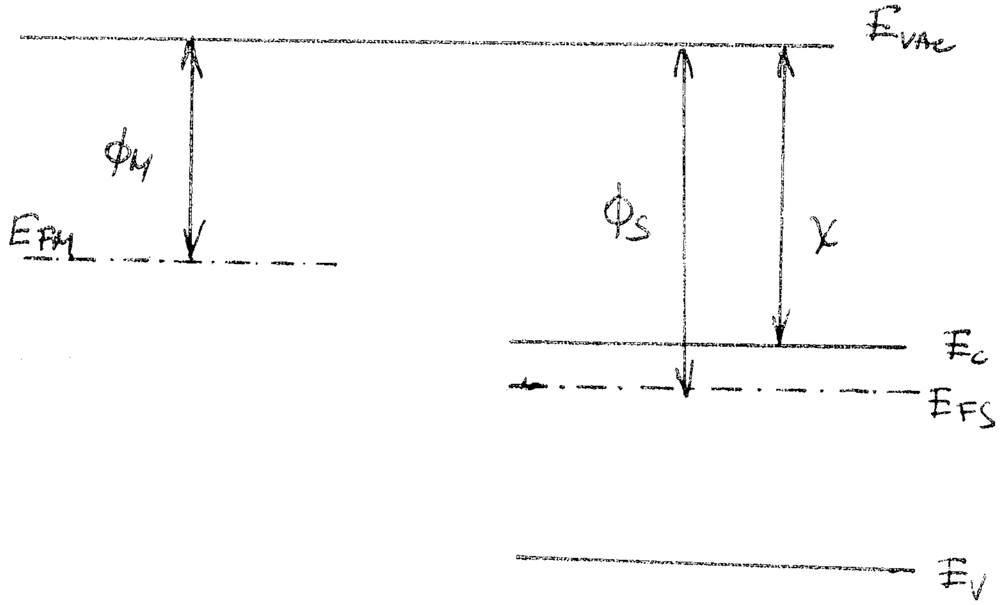
Contact Metal - Semiconductor

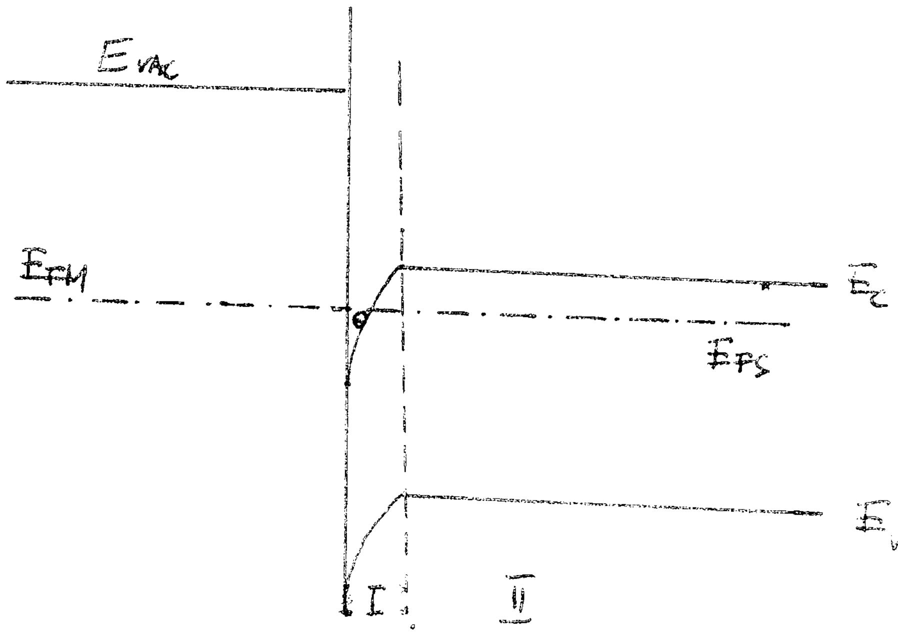
Contact metal - semiconductor represents another excample of inhomogeneous semiconductor structure. After depositing the metal it comes to charge transport between the metal and the semiconductor. As a result of this transfer the semiconductor becomes inhomogeneous. The charge transport and the properties of the M-S structure depend on difference between the work function of Metal and semiconductor and on the type (N or P) of the semiconductor. We will discuss all 4 possibilities and how the M-S structure behaves under bias.

I. N type semiconductor, work function of metal is smaller than work function of the semiconductor ($\phi_M < \phi_S$)

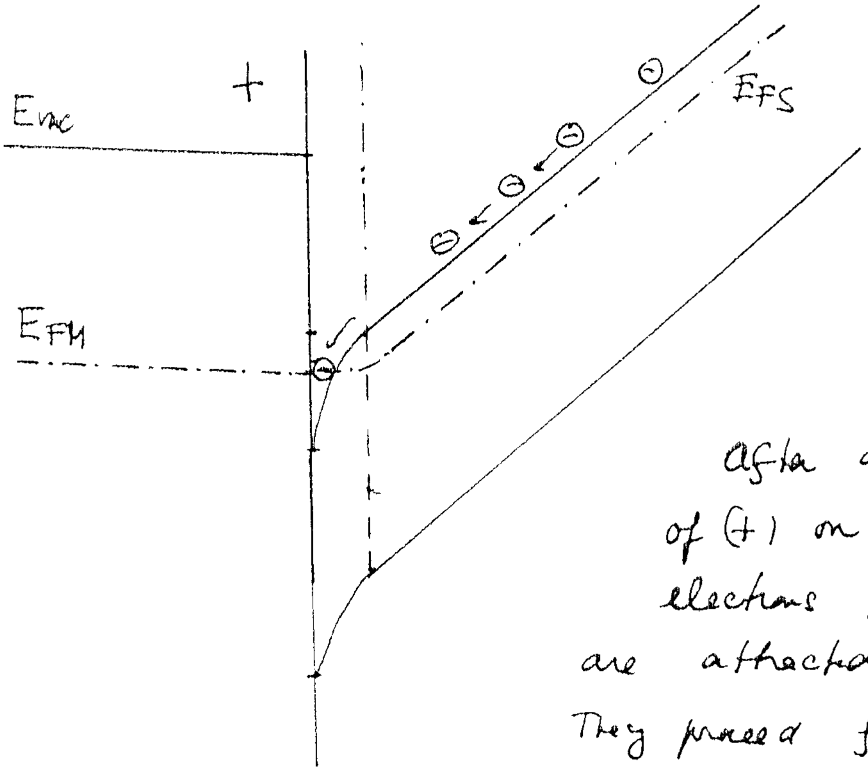
Due to the fact, that $\phi_M < \phi_S$, the Fermi level in the metal is higher at the absolute energy scale, than the Fermi level in the SC ($E_{FM} > E_{FS}$) After joining M and SC, electrons from M are transferred to SC. Because the SC is N-type (electrons are majority carriers), the new electrons from M form a highly conductive, enriched with electrons interface level.

N-type semiconductor , $\phi_M < \phi_S$

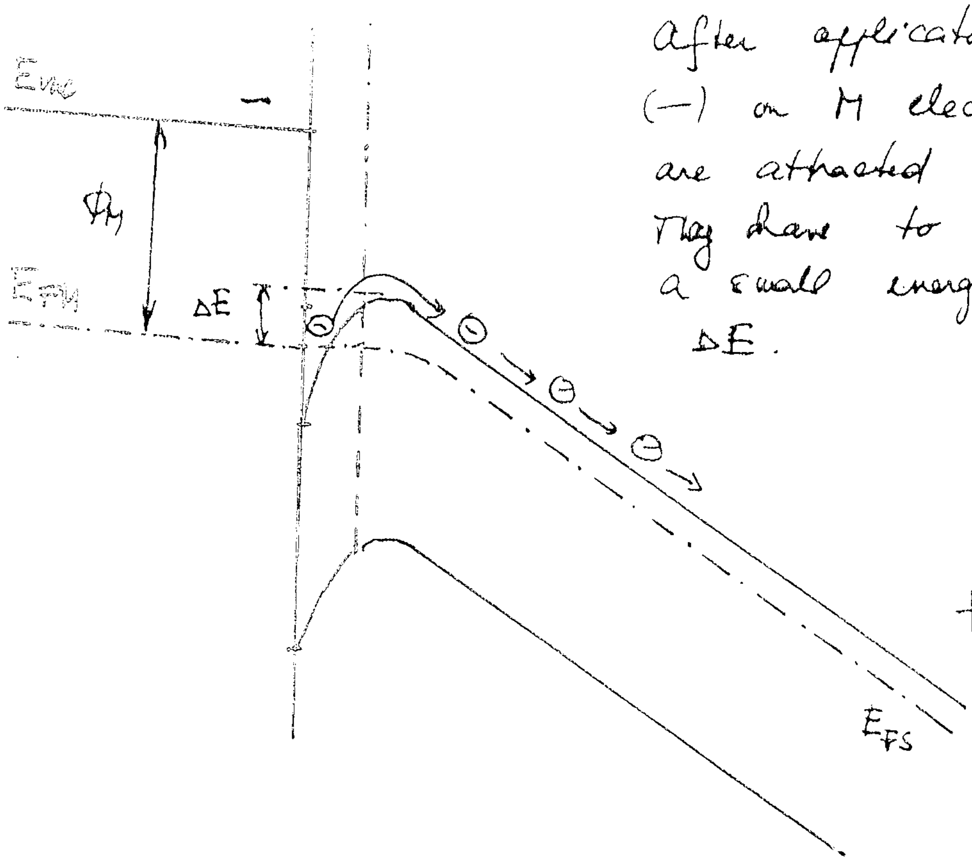




N-type, $\phi_M < \phi_S$ under bias



After application of (+) on metal electrons from SC are attracted to M. They proceed freely, there is no energy barrier

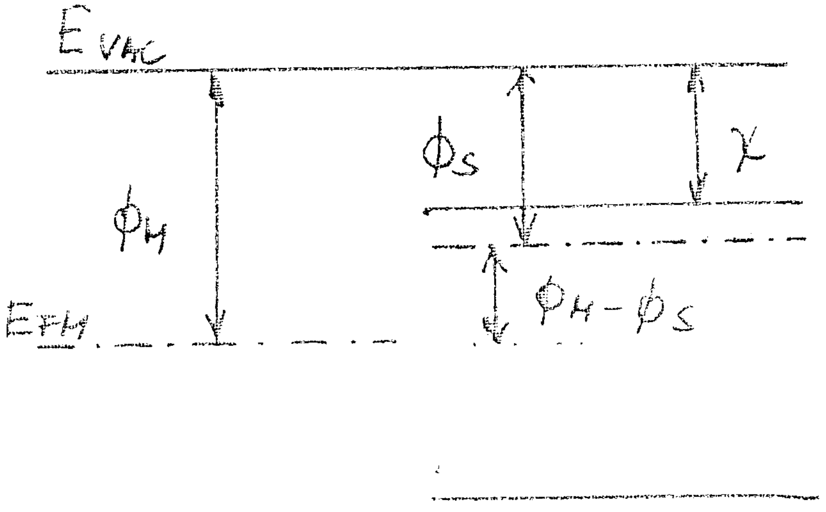


After application of (−) on M electrons are attracted to SC. They have to overcome a small energy barrier ΔE.

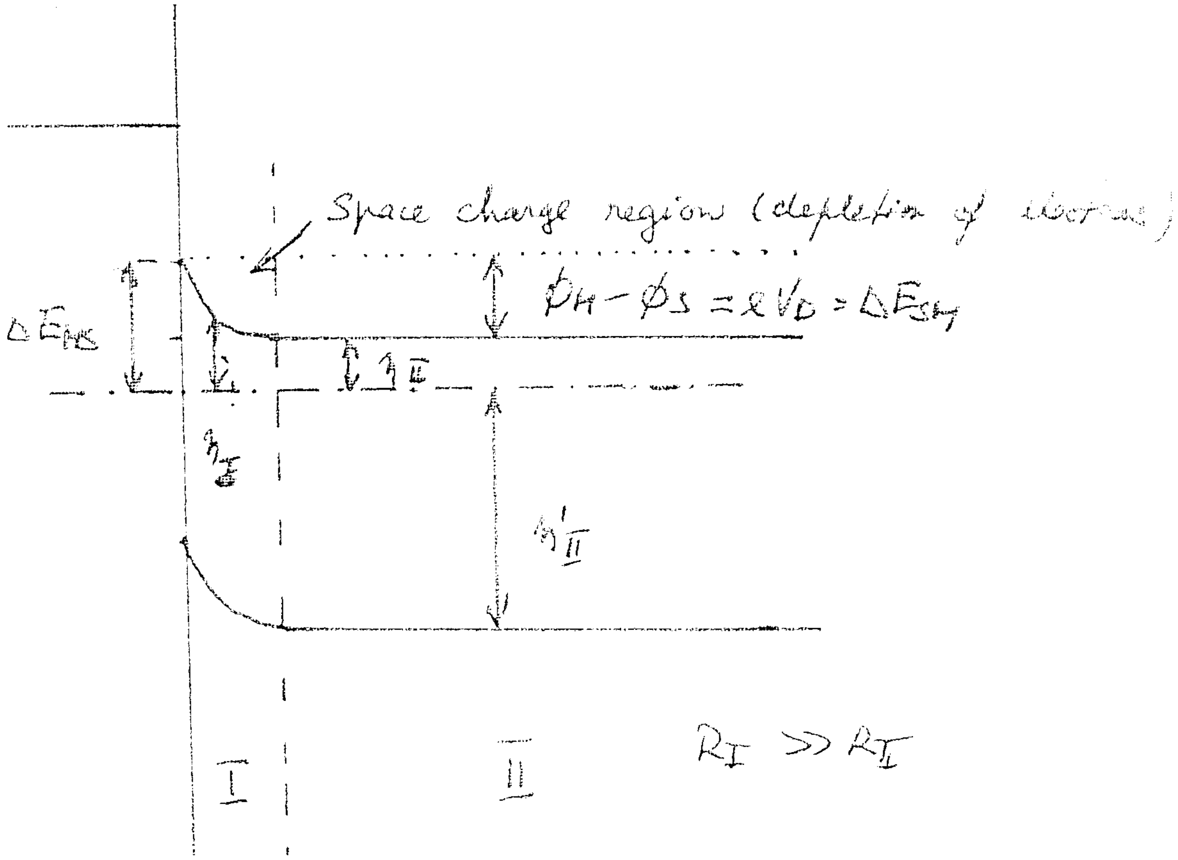
Due to the fact, that there is no or only very small energy barrier, N-type SC with a deposited metal ($\phi_M < \phi_S$) has a linear or nearly linear I-V characteristics.

The metal / semiconductor interface behaves as an ohmic contact.

N-type semiconductor, $\phi_M > \phi_S$



Band scheme before deposition of the metal



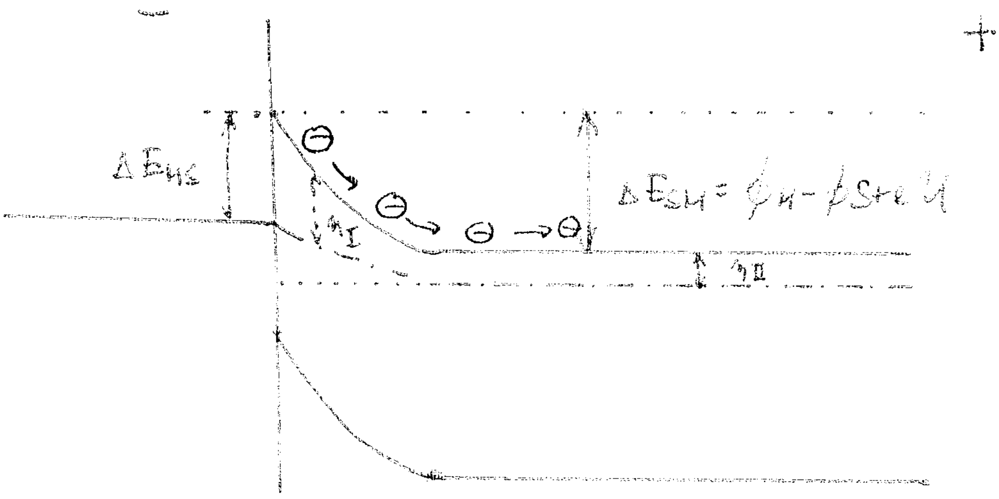
Band scheme after deposition of the metal. Space charge region of uncompensated ionized donors N_D^+ is formed at the interface.

N-type SC, $\Phi_M > \Phi_S$ under bias

The applied bias is almost completely concentrated on the space charge region ($R_I \gg R_{II}$)
$U = (R_I + R_{II}) I \approx R_I I$. The volume of the semiconductor is practically not influenced by the bias. Energy bands are nearly not tilted except of the SCR.

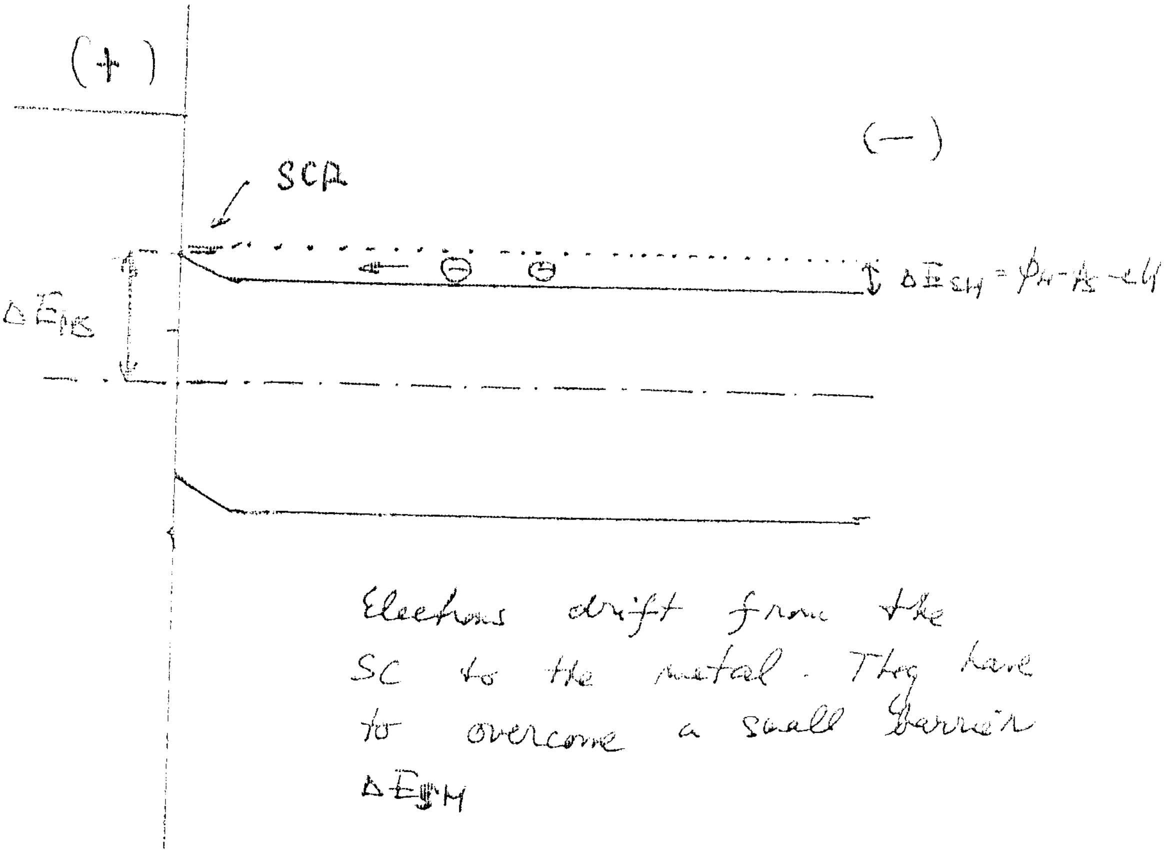
application of (−) on M, (+) on SC

Electrons are attracted to the (+), the width of the SCR increases. Electrons have to overcome the barrier ΔE_{MS} before entering the SC.



The M-S contact is in the reverse direction

The width of the SCR decreases



Electrons drift from the SC to the metal. They have to overcome a small barrier ΔE_{SM}

The M-S contact is in the forward direction

The I-V characteristics is asymmetric, the M-S interface in this case behaves as a rectifying contact and is similar as in case of the p-n junction.