Boltzmann transport equation

The Boltzmann transport equation for free electrons is

$$\frac{\partial f}{\partial t} = -\vec{v}\,\nabla_{\vec{r}} f - \frac{\vec{F}}{m_e}\nabla_{\vec{v}} f + \left\{ \int_{\vec{v}'} W(\vec{v}',\vec{v})\, f(\vec{v}',\vec{r},t) - f(\vec{v},\vec{r},t)\, W(\vec{v},\vec{v}') \right\} d^3v'$$

For case of electrons in crystal lattice we have to modify it

$m_e \rightarrow m_e^*$ (effective mass)

$m_e^*\vec{v} \rightarrow \hbar \vec{k}$ (quasi - impuls)

$\int_{\vec{v}'} \longrightarrow \sum_{k'}$ (the states in the $\vec{k}$ space are quantised as a result of periodic Born - Kármán boundary conditions.)

We also introduce the Lorentz force

$$\vec{F} = -e(\vec{E} + \vec{v}\times\vec{B})$$

We replace $\vec{F}$ with the Lorentz force $\vec{F} = -e(\vec{E} + \vec{v} \times \vec{B})$ and obtain

$$\frac{\partial f}{\partial t} + \vec{v}(\vec{k}) \nabla_{\vec{r}} f - \frac{e}{\hbar} \nabla_{\vec{k}} f \{\vec{E} + \vec{v} \times \vec{B}\} = \left(\frac{\partial f}{\partial t}\right)_{sc}$$

(we have used the eq. $m\, d\vec{v} = \hbar\, d\vec{k}$

$$\Rightarrow \frac{1}{d\vec{v}} = \frac{m}{\hbar} \cdot \frac{1}{d\vec{k}} \;)$$

In the stationary case

$$\vec{v}(\vec{k}) \nabla_{\vec{r}} f - \frac{e}{\hbar} \nabla_{\vec{k}} f \{\vec{E} + \vec{v} \times \vec{B}\} = \left(\frac{\partial f}{\partial t}\right)_{sc}$$

The scattering term can be in case of electrons in the crystal written as

$$\left(\frac{\partial f}{\partial t}\right)_{sc} = \sum_{\vec{k}'} \{ W(\vec{k}', \vec{k}) \underbrace{f(\vec{k}')}_{\text{states occupied by electrons}} \underbrace{(1 - f(\vec{k}))}_{\text{free states}} - W(\vec{k}, \vec{k}') f(\vec{k})(1 - f(\vec{k}')) \}$$

where we have applied the Pauli exclusion principle.

From the principle of detailed balance we conclude, that the number of electrons coming from state $\vec{k}$ to state $\vec{k}'$ as a result of scattering is equal to the number of electrons scattered from $\vec{k}'$ to $\vec{k}$ in equilibrium.

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

In case of elastic scattering $\varepsilon = \varepsilon'$

$\Rightarrow f_0(\varepsilon) = f_0(\varepsilon') \qquad W(\vec{k},\vec{k}') = W(\vec{k}',\vec{k})$

We derived this result for equilibrium conditions. We will assume, that it is valid also out of equilibrium.

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

$$= \sum_{\vec{k}'} W(\vec{k},\vec{k}') \; (f(\vec{k}') - f(\vec{k}))$$

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

↑ non-equilibrium part of f

We will assume, that $f(\vec{k})$ is just $f_0(\vec{k})$ shifted in $\vec{k}$ space as a result of the acting force.

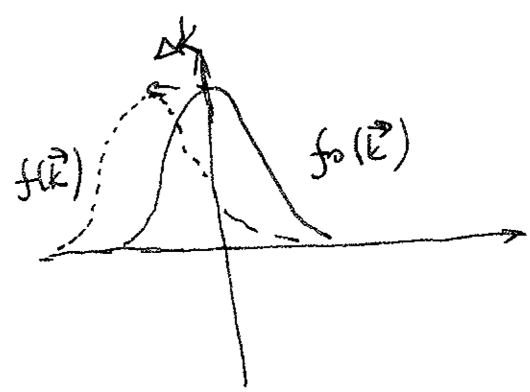
$$f(\vec{k}) = f_0(\vec{k} - \Delta\vec{k}) \qquad \Delta k = \frac{qE\Delta t}{\hbar} = -\frac{eE\Delta t}{\hbar}$$

(From the Drude model)

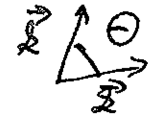
$$f_0(\vec{k} - \Delta\vec{k}) \doteq f_0(\vec{k}) - \frac{\partial f_0}{\partial k}\Delta k = \qquad -\Delta k = \frac{eE\Delta t}{\hbar}$$

$$\doteq f_0(\vec{k}) - \frac{\partial f_0}{\partial \varepsilon}\cdot\frac{\partial \varepsilon}{\partial k}\Delta k$$

(Taylor expansion)



$$\varepsilon = \frac{\hbar^2 k^2}{2m_e^*} \qquad \frac{d\varepsilon}{d\vec{k}} = \frac{\hbar^2 \vec{k}}{m_e^*}$$



θ .. scattering angle

$$f = f_0 - \frac{\partial f_0}{\partial \varepsilon} \cdot \frac{\hbar^2 \Delta \vec{k}}{m_e^*} \cdot \vec{k}$$

$$f(\vec{k}') - f(\vec{k}) = \frac{\partial f_0}{\partial \varepsilon} \cdot \frac{\hbar^2 \Delta \vec{k}}{m_e^*} (\vec{k} - \vec{k}') =$$

$$= \frac{\partial f_0}{\partial \varepsilon} \cdot \frac{\hbar^2 \Delta \vec{k}}{m_e^*} \frac{\vec{k} \cdot \vec{k}}{\vec{k} \cdot \vec{k}} (\vec{k} - \vec{k}') = \frac{\partial f_0}{\partial \varepsilon} \cdot \frac{\hbar^2 \Delta \vec{k}}{m_e^*} \cdot \frac{\vec{k}}{k^2} (k^2 - kk' \cos\theta) =$$

$k = k'$ for elastic scattering

$$= \frac{\partial f_0}{\partial \varepsilon} \cdot \frac{\hbar^2 \Delta \vec{k}}{m_e^*} \vec{k} (1 - \cos\theta)$$

$$\Rightarrow \quad \frac{1}{\tau} = \sum_{\vec{k}'} W(\vec{k}, \vec{k}') (f(\vec{k}') - f(\vec{k})) =$$

$$= \sum_{\vec{k}'} W(\vec{k}, \vec{k}') \underbrace{\frac{\partial f_0}{\partial \varepsilon} \cdot \frac{\hbar^2 \Delta \vec{k}}{m_e^*} \vec{k}}_{-f_1(\vec{k})} (1 - \cos\theta) =$$

$$= - f_1(\vec{k}) \sum_{\vec{k}'} W(\vec{k}, \vec{k}') (1 - \cos\theta)$$

Let us introduce relaxation time

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

We can write

$$\left(\frac{\partial f}{\partial t} \right)_{sc} = - \frac{f_1(\vec{k})}{\tau} = - \frac{(f - f_0)}{\tau}$$

Physical meaning of relaxation time

$$\left(\frac{\partial f}{\partial t}\right)_s = -\frac{(f-f_0)}{\tau}$$

$$\frac{d(f-f_0)}{dt} = -\frac{(f-f_0)}{\tau}$$

$$\frac{d(f-f_0)}{(f-f_0)} = -\frac{dt}{\tau}$$

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

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

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

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

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

relaxation time is a time at which deviation of the distribution function from equilibrium drops to 1/e of its initial value

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

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

where 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.

Matthiessen rule is valid only within the relaxation time approximation (elastic or isotropic scattering)

We switch from summation to integration

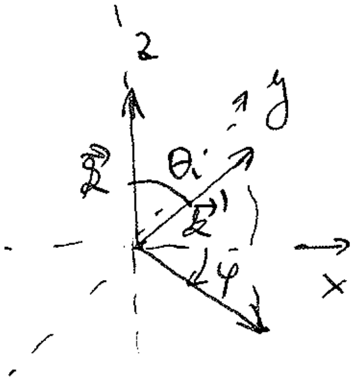
$$\frac{1}{\tau_i} = \frac{V}{(2\pi)^3}\int_{\vec{k}} W_i(\vec{k},\vec{k}')(1-\cos\Theta_i)\,d\vec{k}'$$

We introduce spherical coordinates k, Θ_i and φ

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

(we have chosen the polar axis in the direction of $\vec{k}$, therefore $\Theta_i = \Theta$

scattering angle ↗ ↑ polar angle



Polar axis $\parallel$ to $\vec{k}$

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

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

$\int_0^{2\pi} d\varphi = 2\pi$

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

Fermi golden rule

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

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

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

$$\Psi_k(\vec{r}) = \phi(\vec{r}) \cdot \psi(\vec{r})$$

$\phi(\vec{r})$ ... wave function of the scattering center

$\psi(\vec{r})$ ... wave function of electron

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

$$= \frac{V}{(2\pi)^2}\cdot\frac{1}{\hbar}\int_0^\infty |M_i(\vec{k},\vec{k}')|^2 \delta(\varepsilon-\varepsilon') dk' =$$

$$\varepsilon' = \frac{\hbar^2 k'^2}{2m_e^*} \quad ; \quad k'^2 = \frac{2m_e^*\varepsilon'}{\hbar^2}$$

$$k' = \frac{\sqrt{2m_e^*\varepsilon'}}{\hbar} \qquad dk' = \frac{1}{2\sqrt{\varepsilon'}}\frac{\sqrt{2m_e^*}}{\hbar}d\varepsilon'$$

$$= \frac{V}{(2\pi)^2}\cdot\frac{1}{\hbar}\int_0^\infty |M_i(k,k')|^2 \delta(\varepsilon-\varepsilon')\cdot\frac{(2m_e^*)^{3/2}\varepsilon'}{2\hbar^3}\cdot\frac{1}{\sqrt{\varepsilon'}}\, d\varepsilon' =$$

$$= \frac{V}{(2\pi)^2}\cdot\frac{1}{\hbar}\int_0^\infty |M_i(\vec{k},\vec{k}')|^2 \delta(\varepsilon-\varepsilon')\cdot\frac{(2m_e^*)^{3/2}}{2\hbar^3}\cdot\varepsilon'^{+1/2}d\varepsilon' =$$

We know that the density of states

$$g(\varepsilon') = \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3}\varepsilon'^{1/2}$$

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

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

We assumed that $|M_i(\vec{k},\vec{k}')|$ does not depend on energy

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

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

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

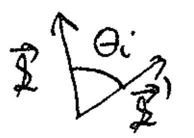
$M_i(\vec{k},\vec{k}')$ for scattering on ionized impurities

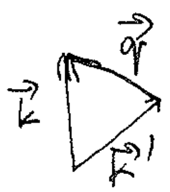
H' for this type of scattering (perturbing potential)

$$H' = H_I' = \pm e\varphi \qquad \varphi = \pm \frac{e}{4\pi\varepsilon_0\varepsilon_r} e^{-\frac{r}{R_S}}$$

Screened Coulomb potential

R_S ... screening length

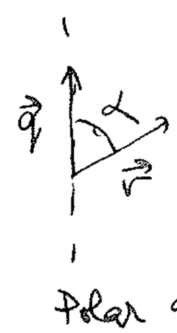




$$q = 2k \sin\frac{\theta_i}{2}$$

We will assume that $\psi_{\vec{k}}(\vec{r})$ is a plane wave

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



Polar axis

.. We have chosen $\vec{q} \parallel z$ as a polar axis

$$\vec{q}\cdot\vec{r} = qr\cos\alpha$$

$$M_I(\vec{k},\vec{k}') = \frac{1}{V}\frac{e^2}{4\pi\varepsilon_0\varepsilon_r}\cdot 2\pi\int_0^\infty\int_0^\pi r e^{-r/R_S} e^{iqr\cos\alpha}\sin\alpha\, d\alpha\, dr =$$

$$= \frac{1}{V}\frac{e^2}{2\varepsilon_0\varepsilon_r}\int_0^\infty r e^{-r/R_S}\int_{+1}^{-1} -e^{iqrt}\,dt\,dr$$

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

$$M_I(\vec{k},\vec{k}') = \frac{1}{V}\frac{e^2}{2\varepsilon_0\varepsilon_r}\int_0^\infty r e^{-r/R_S}\left[\frac{e^{iqrt}}{iqr}\right]_{-1}^{+1} dr =$$

$$= \frac{1}{V}\frac{e^2}{2\varepsilon_0\varepsilon_r}\int_0^\infty r e^{-r/R_S}\left(\frac{e^{iqr}-e^{-iqr}}{iqr}\right) dr =$$

$$= \frac{1}{V}\frac{e^2}{2\varepsilon_0\varepsilon_r}\int_0^\infty r e^{-r/R_S}\frac{2i\sin qr}{iqr}\, dr =$$

$$= \frac{1}{V}\frac{e^2}{\varepsilon_0\varepsilon_r}\int_0^\infty e^{-r/R_S}\sin qr\, dr$$

↑ table integral

$$\int e^{ax}\sin bx\, dx = \frac{e^{ax}}{a^2+b^2}(a\sin bx - b\cos bx)$$

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

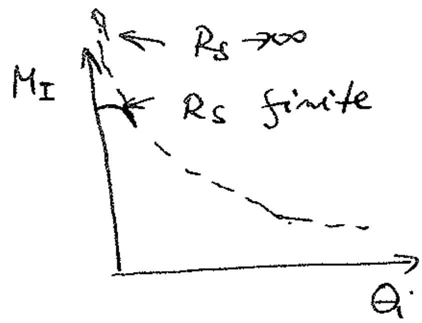
$$M_I(\vec{k},\vec{k}') = \frac{e^2}{V\varepsilon_0\varepsilon_r}\cdot\frac{1}{q}\left[\frac{1}{\left(\frac{1}{R_S}\right)^2+q^2}\left(-\frac{e^{-r/R_S}}{R_S}\sin qr - e^{-r/R_S}q\cos qr\right)\right]_0^\infty$$

$$M_I(\vec{k},\vec{k}') = \frac{e^2}{V\varepsilon_0\varepsilon_r q}\left(\frac{1}{\frac{1}{R_S^2}+q^2}\right)\cdot q = \frac{e^2}{V\varepsilon_0\varepsilon_r}\cdot\frac{1}{\left(\frac{1}{R_S}\right)^2+q^2}$$

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

$\theta_i \to 0 \quad q \to 0$

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



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

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

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

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

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

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

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

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

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

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

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 $a = 1$

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

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

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