

Transport

C:\Program Files\Cornell\SSS\winbin\sommer.exe



quit

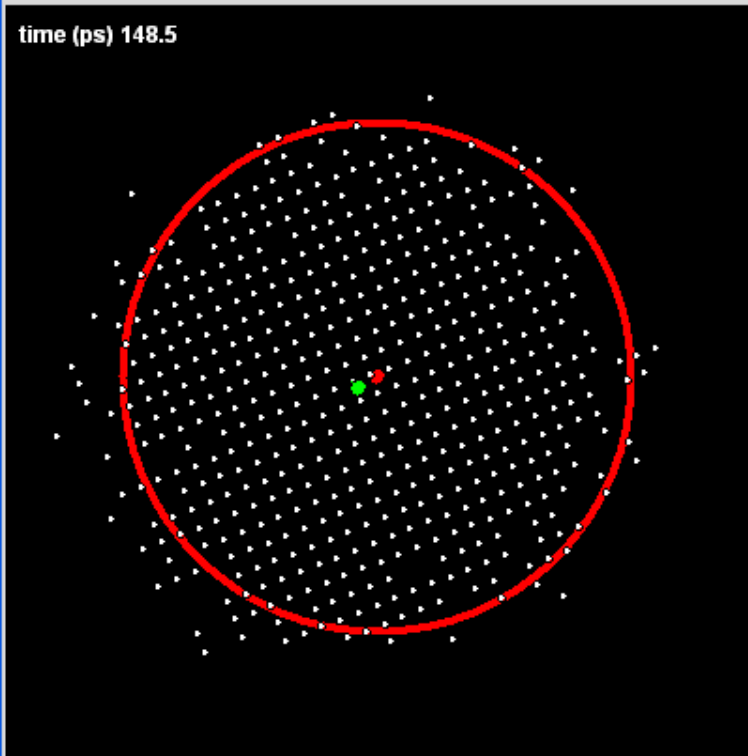
display: large

configure...

presets

help...

time (ps) 148.5



wave vector (1.88, -1.48) 1/Å

stop

initialize

E_x (10⁶ V/m): 1

E_y (10⁶ V/m): 0

B_z (T): 0.9

tau_i (ps): 1.00e+00

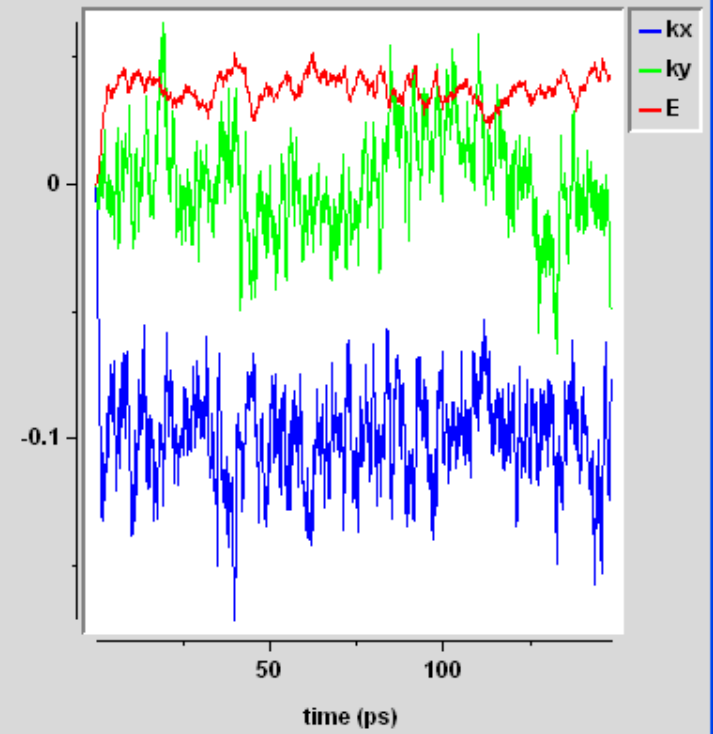
tau_e (ps): 1.00e+04

E_Fermi (eV): 7

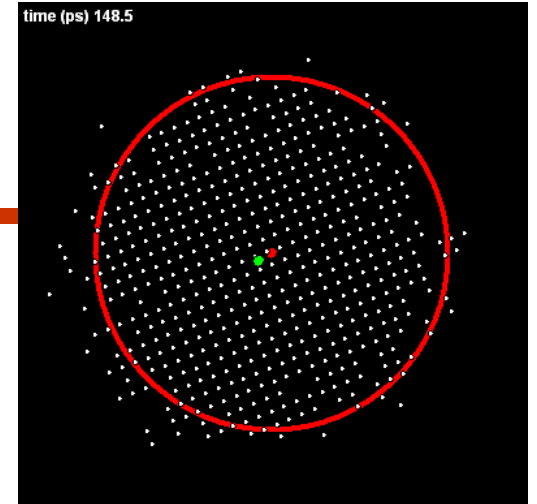
speed: 1

copy graph

$\langle k \rangle$ (1/Å) and E_excess (E_F)



Master equation



$$\vec{j}_{elec} = -e \int \vec{v}(\vec{k}) D(\vec{k}) f(\vec{k}) d\vec{k}$$

$$\frac{d}{dt} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix} = \begin{bmatrix} -\sum_{j \neq 1} \Gamma_{1 \rightarrow j} & \Gamma_{2 \rightarrow 1} & \Gamma_{3 \rightarrow 1} & \Gamma_{4 \rightarrow 1} \\ \Gamma_{1 \rightarrow 2} & -\sum_{j \neq 2} \Gamma_{2 \rightarrow j} & \Gamma_{3 \rightarrow 2} & \Gamma_{4 \rightarrow 2} \\ \Gamma_{1 \rightarrow 3} & \Gamma_{2 \rightarrow 3} & -\sum_{j \neq 3} \Gamma_{3 \rightarrow j} & \Gamma_{4 \rightarrow 3} \\ \Gamma_{1 \rightarrow 4} & \Gamma_{2 \rightarrow 4} & \Gamma_{3 \rightarrow 4} & -\sum_{j \neq 4} \Gamma_{4 \rightarrow j} \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix}$$

Fermi's golden rule:
$$\Gamma_{k \rightarrow k'} = \frac{2\pi}{\hbar} |\langle k' | H | k \rangle|^2 \delta(E_k - E_{k'})$$

Current densities

Electrical $\vec{j}_{\text{elec}} = -e \int \vec{v}_{\vec{k}} D(\vec{k}) f(\vec{k}) d^3 k$

Particle $\vec{j}_n = \int \vec{v}_{\vec{k}} D(\vec{k}) f(\vec{k}) d^3 k$

Energy $\vec{j}_U = \int \vec{v}_{\vec{k}} E(\vec{k}) D(\vec{k}) f(\vec{k}) d^3 k.$

1st law: $dU = dQ - dW + \mu dN.$

Heat $\vec{j}_Q = \int \vec{v}_{\vec{k}} \left(E(\vec{k}) - \mu \right) D(\vec{k}) f(\vec{k}) d^3 k.$

Current densities

Electrical

$$\vec{j}_{\text{elec}} = -e \int \vec{v}_{\vec{k}} D(\vec{k}) f(\vec{k}) d^3 k$$

$$D(\vec{k}) = \frac{2}{(2\pi)^3} \longleftarrow \text{spin}$$

$$\vec{v}_{\vec{k}} = \frac{\nabla_{\vec{k}} E(\vec{k})}{\hbar}$$

$f(\vec{k})$ Probability that state k is occupied.

Liouville's theorem

$f(\vec{r}, \vec{k}, t)$ Probability that state k is occupied at position r and time t .

Number of electrons:
$$N = \int d^3 r \int d^3 k f(\vec{r}, \vec{k}, t).$$

$$\frac{d}{dt} f(\vec{r}, \vec{k}, t) = 0.$$

If the probability of finding an electron at a particular position with a particular momentum decreases, the probability must increase somewhere else.

Boltzmann Equation

$$\frac{d}{dt} f(\vec{r}, \vec{k}, t) = 0.$$

$$\frac{d}{dt} f(\vec{r}, \vec{k}, t) = \frac{\partial f}{\partial x} \frac{dx}{dt} + \frac{\partial f}{\partial y} \frac{dy}{dt} + \frac{\partial f}{\partial z} \frac{dz}{dt} + \frac{\partial f}{\partial k_x} \frac{dk_x}{dt} + \frac{\partial f}{\partial k_y} \frac{dk_y}{dt} + \frac{\partial f}{\partial k_z} \frac{dk_z}{dt} + \frac{\partial f}{\partial t} = 0$$

$$\frac{d}{dt} f(\vec{r}, \vec{k}, t) = \frac{d\vec{r}}{dt} \cdot \nabla_{\vec{r}} f + \frac{d\vec{k}}{dt} \cdot \nabla_{\vec{k}} f + \frac{\partial f}{\partial t} = 0.$$

Crystal momentum $\vec{F}_{\text{ext}} = \hbar \frac{d\vec{k}}{dt}$

$$\frac{\partial f}{\partial t} = -\frac{1}{\hbar} \vec{F}_{\text{ext}} \cdot \nabla_{\vec{k}} f - \vec{v} \cdot \nabla_{\vec{r}} f + \left. \frac{\partial f}{\partial t} \right|_{\text{collisions}}$$

Collision term describes the transitions between k states.

Relaxation time approximation

$$\frac{\partial f}{\partial t} = -\frac{\vec{F}_{ext} \cdot \nabla_k f}{\hbar} - \vec{v} \cdot \nabla f + \left. \frac{\partial f}{\partial t} \right|_{collisions}$$

In the relaxation time approximation,

$$\left. \frac{\partial f}{\partial t} \right|_{collisions} = \frac{f_0(\vec{k}) - f(\vec{k})}{\tau(\vec{k})}$$

If the driving field is turned off, the collision term will drive the system back to equilibrium in time τ .

When $\nabla_k f = \nabla_r f = 0$ and the initial condition is $f = f_1$, the solution to the Boltzmann equation is,

$$f(t) = f_0 + f_1 e^{-t/\tau}$$

Boltzmann equation: relaxation time approx.

The relaxation time approximation:

$$\frac{\partial f}{\partial t} = -\frac{\vec{F}_{ext} \cdot \nabla_k f}{\hbar} - \vec{v} \cdot \nabla f + \frac{f_0(\vec{k}) - f(\vec{k})}{\tau(\vec{k})}$$

in a stationary state $\frac{\partial f}{\partial t} = 0$

If the system is not far from equilibrium, $f \approx f_0$, and we can substitute f_0 for f on the right

$$f(\vec{k}) = f_0(\vec{k}) + \frac{\tau(\vec{k}) \vec{F}_{ext} \cdot \nabla_k f_0}{\hbar} + \tau(\vec{k}) \vec{v} \cdot \nabla f_0$$

$$f_0(\vec{k}) = \frac{1}{\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1}$$

Boltzmann equation: relaxation time approx.

$$f(\vec{k}) \approx f_0(\vec{k}) + \frac{\tau(\vec{k})\vec{F}_{ext} \cdot \nabla_k f_0}{\hbar} + \tau(\vec{k})\vec{v} \cdot \nabla f_0$$

$$\nabla f_0 = \frac{\partial f_0}{\partial T} \nabla T + \frac{\partial f_0}{\partial \mu} \nabla \mu$$

$$f_0(\vec{k}) = \frac{1}{\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1}$$

Temperature and
chemical potential can
depend on position

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

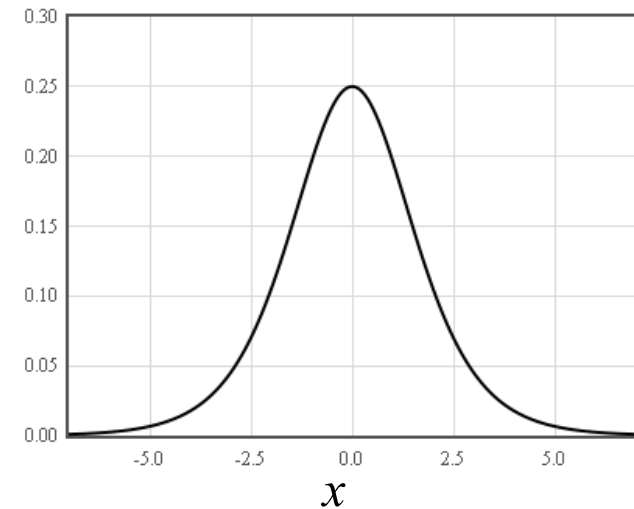
$$f(\vec{k}) \approx f_0(\vec{k}) + \frac{\tau(\vec{k})(-e)(\vec{v} \times \vec{B} + \vec{E}) \cdot \nabla_k f_0}{\hbar} + \tau(\vec{k})\vec{v} \cdot \left(\frac{\partial f_0}{\partial T} \nabla T + \frac{\partial f_0}{\partial \mu} \nabla \mu \right)$$

Temperature gradient

Concentration gradient

Boltzmann equation: relaxation time approx.

$$\frac{\partial f_0}{\partial \mu} = \frac{\frac{1}{k_B T} \exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right)}{\left(\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1\right)^2} = -\frac{\partial f_0}{\partial E} \frac{\exp(x)}{(\exp(x) + 1)^2}$$



$$\begin{aligned} \nabla_k f_0 &= \frac{\frac{-1}{k_B T} \exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right)}{\left(\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1\right)^2} \nabla_k E(\vec{k}) \\ &= \frac{\partial f_0}{\partial E} \nabla_k E(\vec{k}) \end{aligned}$$

$$\begin{aligned} \frac{\partial f_0}{\partial T} &= \frac{\frac{E(\vec{k}) - \mu}{k_B T^2} \exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right)}{\left(\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1\right)^2} \\ &= -\frac{\partial f_0}{\partial E} \frac{E(\vec{k}) - \mu}{T} \end{aligned}$$

Only the states near the Fermi surface contribute.

Boltzmann equation: relaxation time approx.

$$f(\vec{k}, \vec{r}) \approx f_0(\vec{k}, \vec{r}) - \frac{\tau(\vec{k})}{\hbar} \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \cdot \left(e\vec{E} + \nabla_{\vec{r}} \mu + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right)$$

$$\vec{j}_{elec} = -e \int \vec{v}(\vec{k}) D(\vec{k}) f(\vec{k}) d\vec{k}$$

density of states $D(\vec{k}) = \frac{2^{\text{spin}}}{(2\pi)^3}$

$$\vec{j}_{elec} = -\frac{e}{4\pi^3 \hbar} \int \nabla_{\vec{k}} E(\vec{k}) \left(f_0(\vec{k}, \vec{r}) - \frac{\tau(\vec{k})}{\hbar} \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \cdot \left(e\vec{E} + \nabla_{\vec{r}} \mu + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3k.$$

The contribution of $f_0(k)$ is zero

Current densities

$$\vec{j}_{\text{elec}} = -e \int \vec{v}_{\vec{k}} D(\vec{k}) f(\vec{k}) d^3 k$$

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3 \hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(e\vec{E} + \nabla_{\vec{r}} \mu + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3 k.$$

$$\vec{j}_n = \int \vec{v}_{\vec{k}} D(\vec{k}) f(\vec{k}) d^3 k.$$

$$\vec{j}_n = -\frac{1}{4\pi^3 \hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(e\vec{E} + \nabla_{\vec{r}} \mu + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3 k$$

$$\vec{j}_U = \int \vec{v}_{\vec{k}} E(\vec{k}) D(\vec{k}) f(\vec{k}) d^3 k.$$

$$\vec{j}_U = -\frac{1}{4\pi^3 \hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} E(\vec{k}) \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(e\vec{E} + \nabla_{\vec{r}} \mu + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3 k.$$

$$\vec{j}_Q = \int \vec{v}_{\vec{k}} (E(\vec{k}) - \mu) D(\vec{k}) f(\vec{k}) d^3 k$$

$$\vec{j}_Q = -\frac{1}{4\pi^3 \hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} (E(\vec{k}) - \mu) \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(e\vec{E} + \nabla_{\vec{r}} \mu + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3 k.$$

Electrochemical potential

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(e\vec{E} + \nabla_{\vec{r}}\mu + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}}T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3k$$

The electrochemical potential $\tilde{\mu} = -e\phi + \mu$
is what a voltmeter measures

ϕ is the electrostatic potential
 μ is the chemical potential

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\nabla_{\vec{r}}\tilde{\mu} + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}}T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3k.$$

Electrical conductivity

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\nabla_{\vec{r}} \tilde{\mu} + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3k.$$

no temperature gradient or magnetic field

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \nabla_{\vec{r}} \tilde{\mu} \right) d^3k.$$

$$\begin{bmatrix} j_x \\ j_y \\ j_z \end{bmatrix} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} \qquad \begin{bmatrix} j_x \\ j_y \\ j_z \end{bmatrix} = e \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} \begin{bmatrix} \frac{\partial \tilde{\mu}}{\partial x} \\ \frac{\partial \tilde{\mu}}{\partial y} \\ \frac{\partial \tilde{\mu}}{\partial z} \end{bmatrix}$$

Electrical conductivity

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \nabla_{\vec{r}} \tilde{\mu} \right) d^3k.$$

$$\begin{bmatrix} j_x \\ j_y \\ j_z \end{bmatrix} = e \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} \begin{bmatrix} \frac{\partial \tilde{\mu}}{\partial x} \\ \frac{\partial \tilde{\mu}}{\partial y} \\ \frac{\partial \tilde{\mu}}{\partial z} \end{bmatrix}$$

$$\sigma_{ij} = \frac{e^2}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \cdot \hat{e}_i \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \hat{e}_j \right) d^3k$$

for cubic crystals:

$$\sigma = \frac{e^2}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \hat{z} \right)^2 d^3k$$

Free-electron model: electrical conductivity

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m^*}, \quad \nabla_{\vec{k}} E(\vec{k}) = \frac{\hbar^2}{m^*} (k_x \hat{x} + k_y \hat{y} + k_z \hat{z})$$

$$\sigma = \frac{e^2}{4\pi^3 \hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \hat{z} \right)^2 d^3 k$$

assuming a single lifetime τ

$$\sigma = \frac{\hbar^2 e^2 \tau}{4\pi^3 m^{*2}} \int \frac{\partial f_0}{\partial \mu} k_z^2 d^3 k.$$

Free-electron model: electrical conductivity

$$\sigma = \frac{\hbar^2 e^2 \tau}{4\pi^3 m^{*2}} \int \frac{\partial f_0}{\partial \mu} k_z^2 d^3 k.$$

The differential volume is,

$$d^3 k = k^2 \sin \theta dk d\theta d\varphi \quad k_z = k \cos \theta,$$

$$\sigma = \frac{\hbar^2 e^2 \tau}{4\pi^3 m^{*2}} \int \frac{\partial f_0}{\partial \mu} k^4 \cos^2 \theta \sin \theta dk d\theta d\varphi.$$

The integral over φ contributes a factor of 2π .

$$\sigma = \frac{\hbar^2 e^2 \tau}{2\pi^2 m^{*2}} \int \frac{\partial f_0}{\partial \mu} k^4 \cos^2 \theta \sin \theta dk d\theta.$$

The integral over θ contributes a factor of $2/3$.

$$\sigma = \frac{\hbar^2 e^2 \tau}{3\pi^2 m^{*2}} \int \frac{\partial f_0}{\partial \mu} k^4 dk.$$

Free-electron model: electrical conductivity

$$\sigma = \frac{\hbar^2 e^2 \tau}{3\pi^2 m^{*2}} \int \frac{\partial f_0}{\partial \mu} k^4 dk.$$

The derivative of the Fermi function is,

$$\frac{\partial f_0}{\partial \mu} = \frac{\exp(x)}{k_B T (\exp(x) + 1)^2}$$

where

$$x = \frac{E - \mu}{k_B T} = \frac{\frac{\hbar^2}{2m^*} (k^2 - k_F^2)}{k_B T},$$

and $\mu = \hbar^2 k_F^2 / 2m^*$. Differentiating to find dk

$$dk = \frac{m^* k_B T}{\hbar^2 k} dx$$

The conductivity can be written as,

$$\sigma = \frac{e^2 \tau}{3\pi^2 m^*} \int \frac{\exp(x)}{(\exp(x) + 1)^2} k^3 dx.$$

Free-electron model: electrical conductivity

$$\sigma = \frac{e^2 \tau}{3\pi^2 m^*} \int \frac{\exp(x)}{(\exp(x) + 1)^2} k^3 dx.$$

k is approximately k_F and it can be pulled out of the integral.
The remaining integral over x evaluates to 1

$$\sigma = \frac{e^2 \tau k_F^3}{3\pi^2 m^*}.$$

For free electrons,

$$n = \frac{k_F^3}{3\pi^2}.$$

In terms of the electron density, the electrical conductivity is,

$$\sigma = \frac{ne^2 \tau}{m^*}.$$

Thermoelectric current

A temperature gradient can cause a current to flow along a wire. The electrons move from the hot side to the cold side. Both charge and energy are transported in this case. The general expression for the electric current density is,

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\nabla_{\vec{r}} \tilde{\mu} + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3 k.$$

No magnetic field is applied. One end of the wire is grounded and the other is attached to an ammeter which is then also grounded. There is no voltage drop across a perfect ammeter so the gradient of the electrochemical potential is zero. The thermoelectric current produced by this temperature gradient is,

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T \right) \right) d^3 k.$$

Thermal conductivity

The electrons carry heat as well as charge.

$$\vec{j}_Q = -\frac{1}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left(E(\vec{k}) - \mu \right) \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T \right) \right) d^3 k.$$

Generally, the relationship between the thermal current density and the temperature gradient is described by the thermal conductivity matrix,

$$\begin{bmatrix} j_{Qx} \\ j_{Qy} \\ j_{Qz} \end{bmatrix} = - \begin{bmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix} \begin{bmatrix} \frac{\partial T}{\partial x} \\ \frac{\partial T}{\partial y} \\ \frac{\partial T}{\partial z} \end{bmatrix}.$$

The thermal conductivity matrix can be calculated from the dispersion relation as,

$$K_{ij} = \frac{1}{4\pi^3\hbar^2 T} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left(E(\vec{k}) - \mu \right) \nabla_{\vec{k}} E(\vec{k}) \cdot \hat{e}_i \left(E(\vec{k}) - \mu \right) \nabla_{\vec{k}} E(\vec{k}) \cdot \hat{e}_j d^3 k.$$

Here \hat{e}_i are the unit vectors $i = [x, y, z]$. For cubic crystals the thermal conductivity is a constant,

$$K = \frac{1}{4\pi^3\hbar^2 T} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left(\left(E(\vec{k}) - \mu \right) \nabla_{\vec{k}} E(\vec{k}) \cdot \hat{z} \right)^2 d^3 k.$$

Thermoelectric current

$$K = \frac{1}{4\pi^3 \hbar^2 T} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left((E(\vec{k}) - \mu) \nabla_{\vec{k}} E(\vec{k}) \cdot \hat{z} \right)^2 d^3 k.$$

(Similar calculation as before, See notes)

The electrical contribution to the thermal conductivity in the free electron model is,

$$K = \frac{\pi^2 \tau n k_B^2 T}{3m^*}.$$

Free-electron model: Wiedemann–Franz law

$$\frac{K}{\sigma} = LT.$$

Here K is the electrical component of the thermal conductivity, σ is the thermal conductivity, T is the absolute temperature, and L is the Lorentz number. For the free-electron model, the electrical and thermal conductivities are,

$$\sigma = \frac{ne^2\tau}{m^*} \quad K = \frac{\pi^2\tau nk_B^2 T}{3m^*}.$$

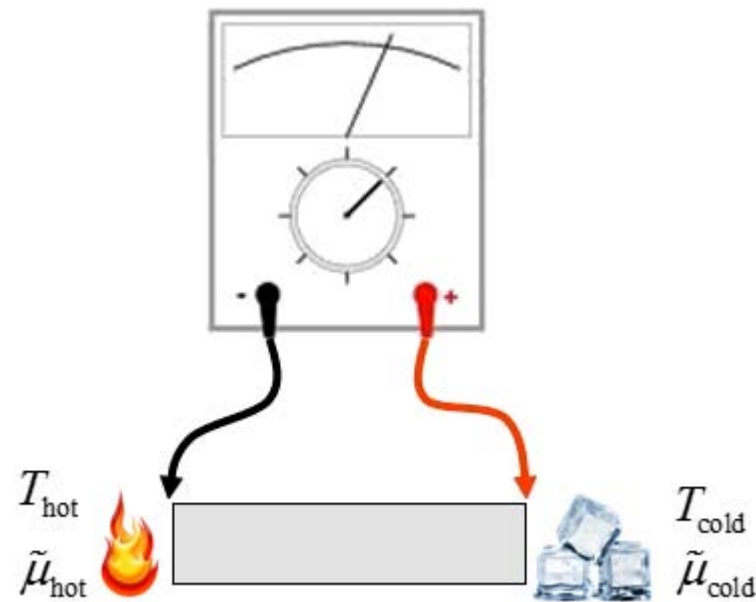
The Lorentz number for free electrons is,

$$L = \frac{\pi^2 k_B^2}{3e^2} = 2.44 \times 10^{-8} \text{ W } \Omega \text{ K}^{-2}.$$

Generally, both K and σ are matrices so when the crystal does not have a high symmetry, the general relationship between them would be described by a fourth-rank tensor.

Seebeck effect

$$\nabla_{\vec{r}} \tilde{\mu} = -S \nabla_{\vec{r}} T.$$



$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3 \hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\nabla_{\vec{r}} \tilde{\mu} + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3 k$$

$$\vec{j}_{\text{elec}} = 0$$

$$\vec{B} = 0$$

Seebeck effect

$$0 = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \cdot \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\nabla_{\vec{r}} \tilde{\mu} + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T \right) \right) d^3k.$$

$$\begin{bmatrix} \frac{\partial \tilde{\mu}}{\partial x} \\ \frac{\partial \tilde{\mu}}{\partial y} \\ \frac{\partial \tilde{\mu}}{\partial z} \end{bmatrix} = - \begin{bmatrix} S_{xx} & S_{xy} & S_{xz} \\ S_{yx} & S_{yy} & S_{yz} \\ S_{zx} & S_{zy} & S_{zz} \end{bmatrix} \begin{bmatrix} \frac{\partial T}{\partial x} \\ \frac{\partial T}{\partial y} \\ \frac{\partial T}{\partial z} \end{bmatrix}$$

$$0 = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \cdot \hat{e}_i \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\begin{pmatrix} -S_{xj} \\ -S_{yj} \\ -S_{zj} \end{pmatrix} + \frac{E(\vec{k}) - \mu}{T} \hat{e}_j \right) \right) d^3k$$

Thermal conductivity again

$$T_1 \quad \boxed{\hspace{10em}} \quad T_2$$

Open boundary conditions

A heat current will also flow in this case. The expression for the heat current is,

$$\vec{j}_Q = -\frac{1}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} (E(\vec{k}) - \mu) \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\nabla_{\vec{r}} \tilde{\mu} + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T \right) \right) d^3k.$$

In this experiment, the electrochemical potential and the temperature gradient are related by $\nabla_{\vec{r}} \tilde{\mu} = -S \nabla_{\vec{r}} T$ so this is inserted into the expression for the heat current.

$$\vec{j}_Q = -\frac{1}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} (E(\vec{k}) - \mu) \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(-S \nabla_{\vec{r}} T + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T \right) \right) d^3k.$$

The thermal conductivity in this case is,

$$K_{ij} = -\frac{1}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} (E(\vec{k}) - \mu) \nabla_{\vec{k}} E(\vec{k}) \cdot \hat{e}_i \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(-S \hat{e}_j + \frac{E(\vec{k}) - \mu}{T} \hat{e}_j \right) \right) d^3k.$$

new term

Thermoelectric effects

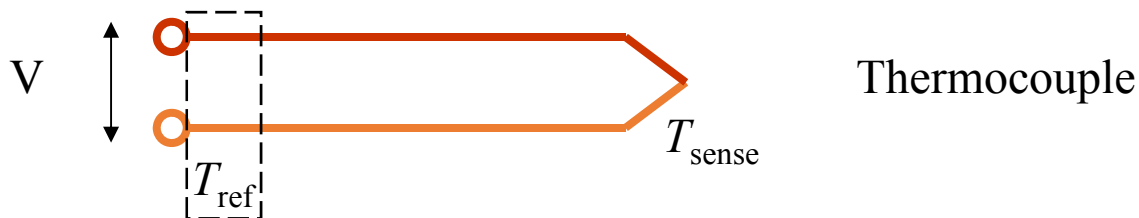
Seebeck effect:

A thermal gradient causes a thermal current to flow. This results in a voltage which sends the low entropy charge carriers back to the hot end.

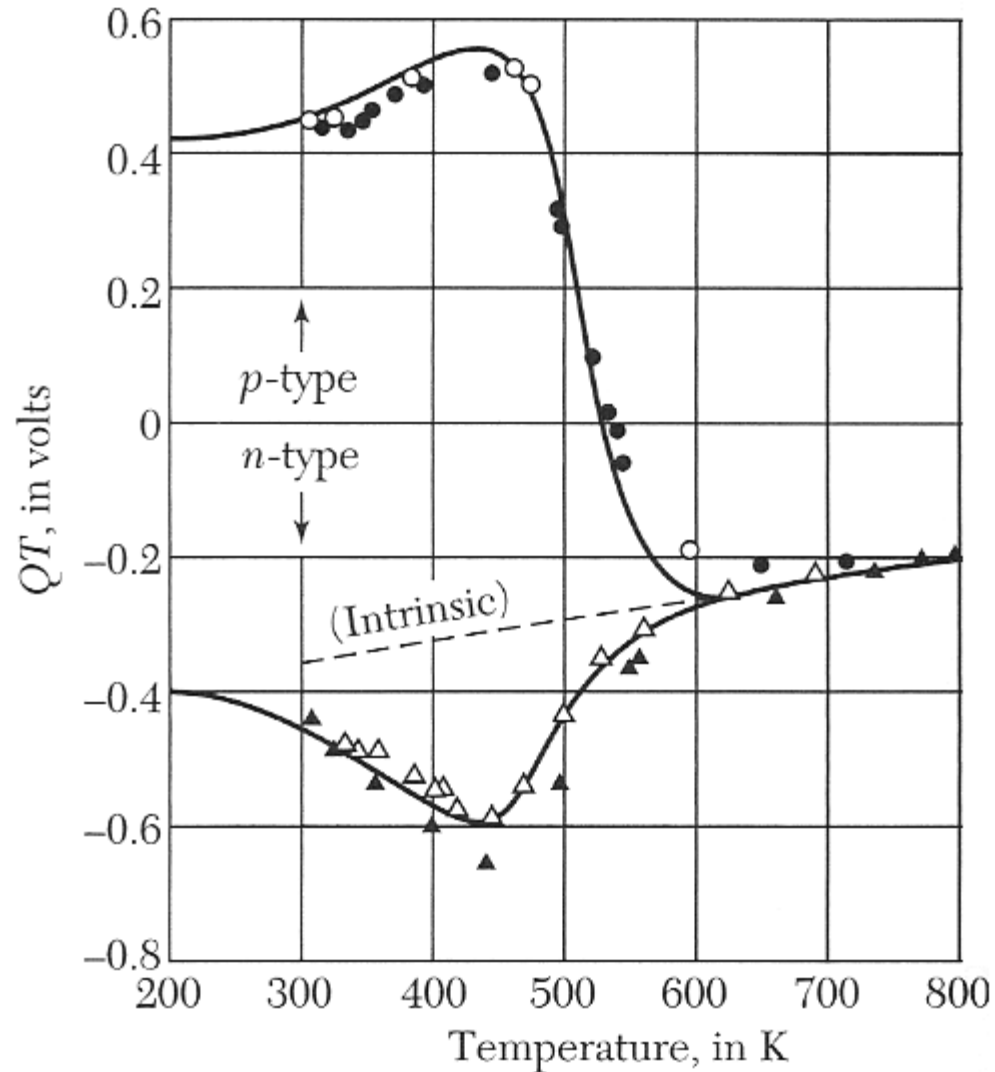
$$\nabla \tilde{\mu} = -S \nabla T$$

S is the absolute thermal power (often also called Q). The sign of the voltage (electrochemical potential, electromotive force) is the same as the sign of the charge carriers.

The Seebeck effect can be used to make a thermometer. The gradient of the temperature is the same along both wires but the gradient in electrochemical potential differs.



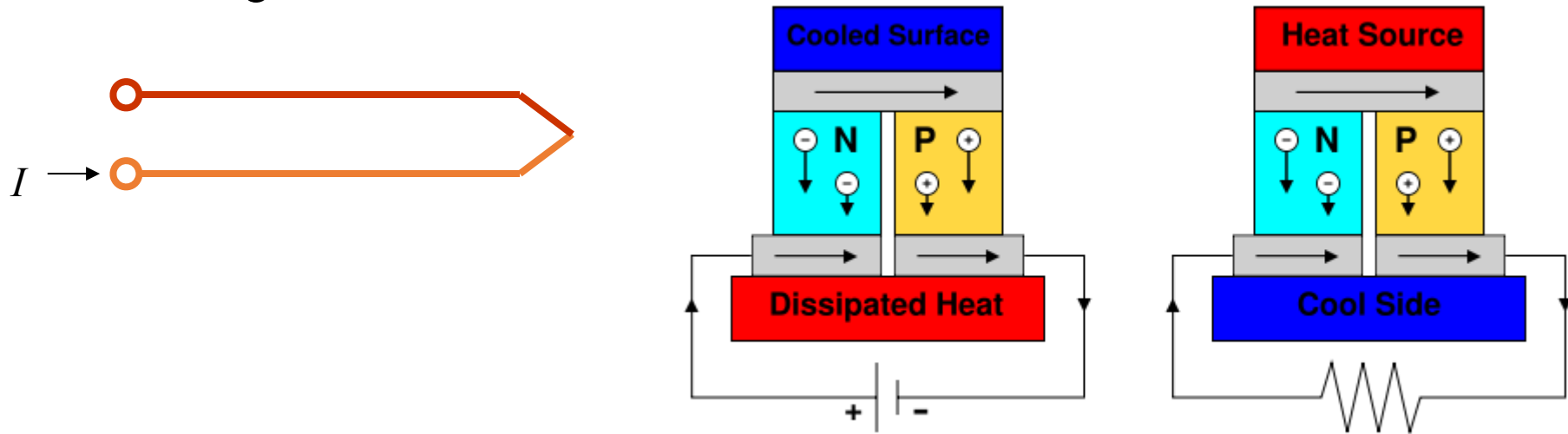
Thermoelectric effects



Intrinsic Q is negative because electrons have a higher mobility.

Thermoelectric effects

Peltier effect: driving a through a bimetallic junction causes heating or cooling.



Cooling takes place when the electrons make a transition from low entropy to high entropy at the junction.

Bismuth chalcogenides Bi_2Te_3 and Bi_2Se_3

Hall effect

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\nabla_{\vec{r}} \tilde{\mu} + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3k.$$

$$\nabla_{\vec{r}} T = 0$$

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\nabla_{\vec{r}} \tilde{\mu} + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3k.$$

$$R_{lmn} = \frac{\nabla_{\vec{r}} \tilde{\mu}_l}{e j_m B_n}.$$

$$R_{lmn} = \left[\frac{e^2}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \cdot \hat{e}_m \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\hat{e}_l + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \hat{e}_n \right) \right) d^3k \right]^{-1}.$$

Nerst effect

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\nabla_{\vec{r}} \tilde{\mu} + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3k.$$

$$\vec{j}_{\text{elec}} = 0$$

$$0 = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\nabla_{\vec{r}} \tilde{\mu} + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3k.$$

$$N_{lmn} = \frac{\nabla \tilde{\mu}_l}{e \nabla T_m B_n}$$

$$0 = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \cdot \hat{e}_i \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\begin{pmatrix} eN_{xyz} \\ eN_{yyz} \\ eN_{zzz} \end{pmatrix} + \frac{E(\vec{k}) - \mu}{T} \hat{y} + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \hat{z} \right) \right) d^3k.$$

Annalen der Physik, vol. 265, pp. 343–347, 1886

***IX. Ueber das Auftreten electromotorischer Kräfte
in Metallplatten, welche von einem Wärmestrome
durchflossen werden und sich im magnetischen
Felde befinden;***

von A. v. Ettingshausen und stud. W. Nernst.

(Aus d. Anz. d. k. Acad. d. Wiss. in Wien, mitgetheilt von den Herren Verf.)

Bei Gelegenheit der Beobachtung des Hall'schen Phänomens im Wismuth wurden wir durch gewisse Unregelmässigkeiten veranlasst, folgenden Versuch anzustellen.

Eine rechteckige Wismuthplatte, etwa 5 cm lang, 4 cm breit, 2 mm dick, mit zwei an den längeren Seiten einander gegenüber liegenden Electroden versehen, ist in das Feld eines Electromagnets gebracht, sodass die Kraftlinien die Ebene der Platte senkrecht schneiden; dieselbe wird durch federnde Kupferbleche getragen, in welche sie an den kürzeren Seiten eingeklemmt ist, jedoch geschützt vor directer metallischer Berührung mit dem Kupfer durch zwischengelegte Glimmerblätter.

Etingshausen effect

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\nabla_{\vec{r}} \tilde{\mu} + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3k.$$

The sample is electrically grounded so $\nabla_{\vec{r}} \tilde{\mu} = 0$.

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2} \int \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \left(\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3k.$$

Boltzmann Group



Albert von Ettingshausen,
Prof. at TU
Graz.



Nernst was a student of Boltzmann and von Ettingshausen. He won the 1920 Nobel prize in Chemistry.

(Standing, from the left) Walther Nernst, Heinrich Streintz, Svante Arrhenius, Hiecke, (sitting, from the left) Aulinger, Albert von Ettingshausen, Ludwig Boltzmann, Ignacij Klemencic, Hausmanninger (1887).

Thermoelectric effects

$$f(\vec{k}, \vec{r}) \approx f_0(\vec{k}, \vec{r}) - \frac{\tau(\vec{k})}{\hbar} \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \cdot \left(\nabla_{\vec{r}} \tilde{\mu} + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right)$$

Electrical current: $\vec{j}_{elec} = \frac{-e}{4\pi^3} \int v(\vec{k}) f(\vec{k}) d^3 k$

Particle current: $\vec{j}_n = \frac{1}{4\pi^3} \int v(\vec{k}) f(\vec{k}) d^3 k$

Energy current: $\vec{j}_E = \frac{1}{4\pi^3} \int v(\vec{k}) E(\vec{k}) f(\vec{k}) d^3 k$

Heat current: $\vec{j}_Q = \frac{1}{4\pi^3} \int v(\vec{k}) (E(\vec{k}) - \mu) f(\vec{k}) d^3 k$

Thermoelectric effects

Electrical conductivity: $\sigma_{mn} = \frac{j_{em}}{E_n}$ $\nabla T = 0, \vec{B} = 0$

Thermal conductivity: $\kappa_{mn} = \frac{-j_{Qm}}{\nabla T_n}$ $\vec{B} = 0$

Peltier coefficient: $\Pi_{mn} = \frac{j_{Qm}}{j_{en}}$ $\nabla T = 0, \vec{B} = 0$

Thermopower (Seebeck effect): $S_{mn} = \frac{-\nabla \tilde{\mu}_m}{\nabla T_n}$ $\vec{j}_e = 0, \vec{B} = 0$

Hall effect: $R_{lmn} = \frac{E_l}{j_{em} B_n}$ $\nabla T = 0, j_{el} = 0$

Nerst effect: $N_{lmn} = \frac{E_l}{B_m \nabla T_n}$ $j_{elec} = 0$

Bloch waves in 1-D

Consider an electron moving in a periodic potential $V(x)$. The period of the potential is a , $V(x + a) = V(x)$. The Schrödinger equation for this case is,

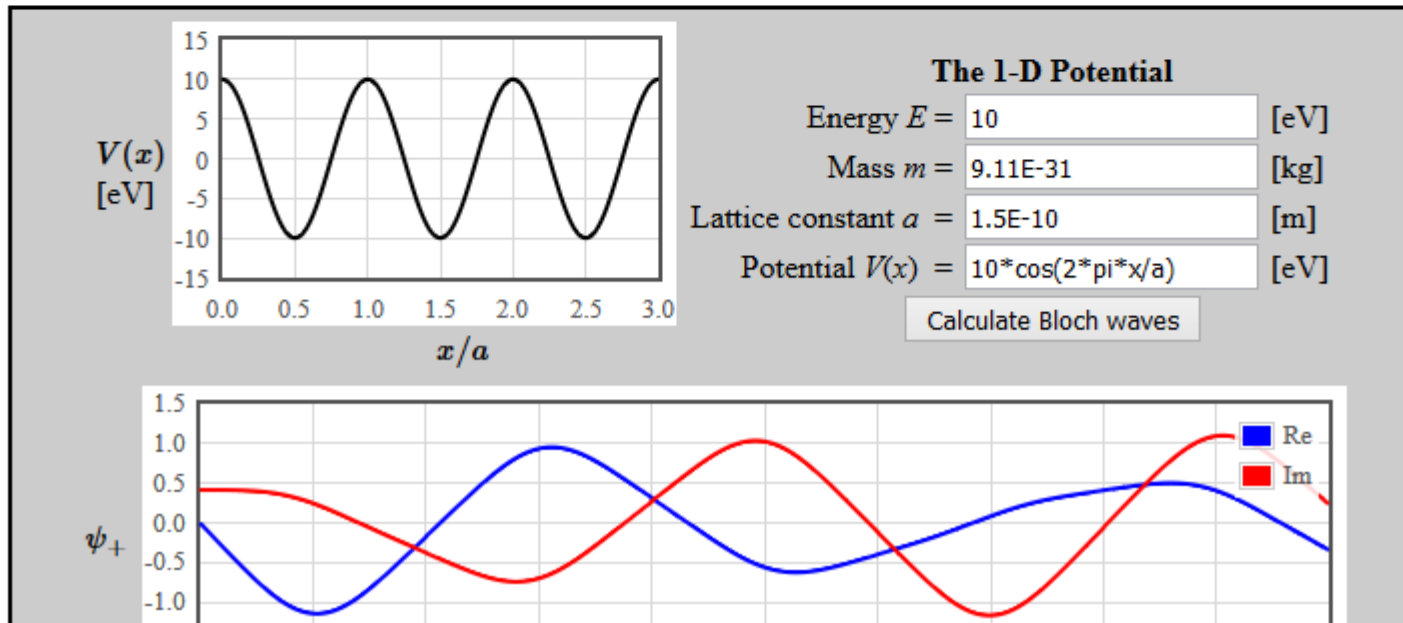
$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi. \quad (1)$$

Quantum mechanically, the electron moves as a wave through the potential. Due to the diffraction of these waves, there are bands of energies where the electron is allowed to propagate through the potential and bands of energies where no propagating solutions are possible. The Bloch theorem states that the propagating states have the form,

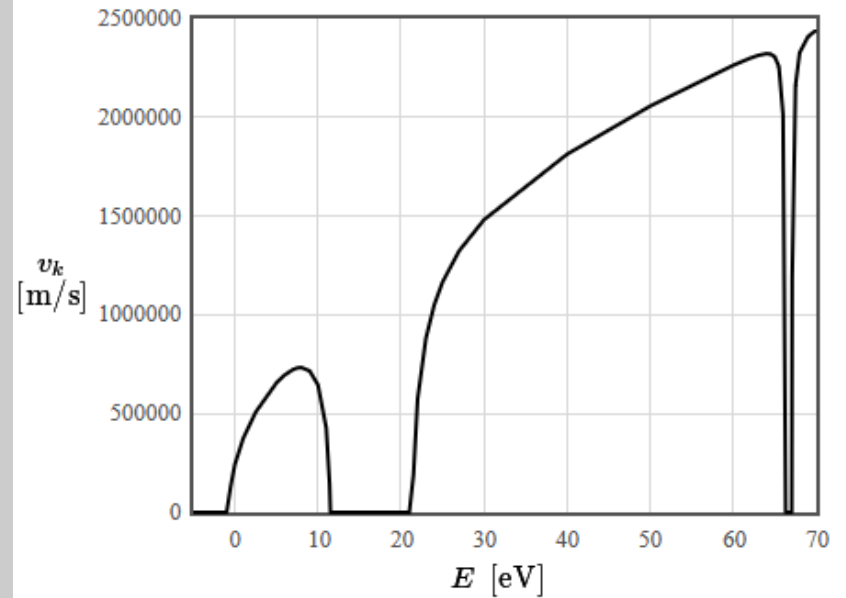
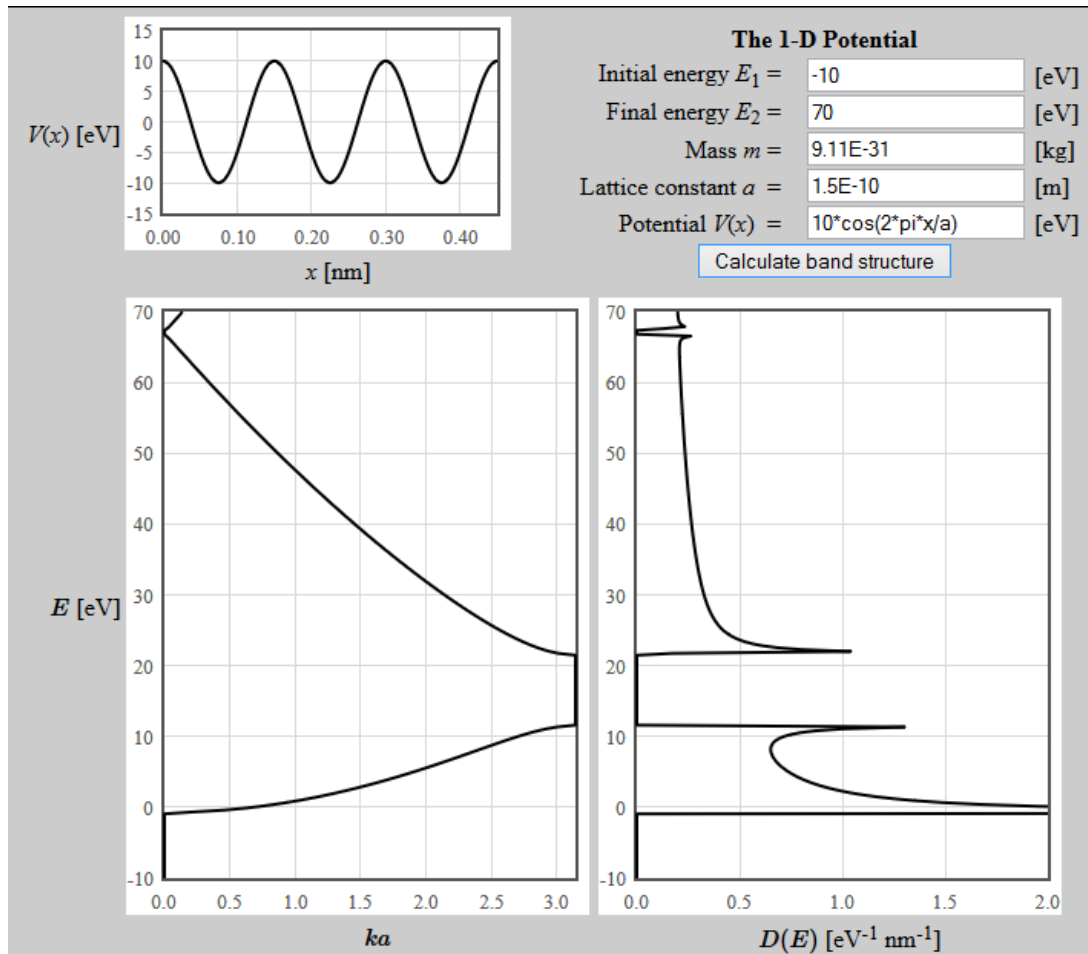
$$\psi = e^{ikx} u_k(x). \quad (2)$$

where k is the wavenumber and $u_k(x)$ is a periodic function with periodicity a .

There is a left moving Bloch wave $\psi_- = e^{-ikx} u_{k-}$ and a right moving Bloch wave $\psi_+ = e^{ikx} u_{k+}$ for every energy. The following form calculates the Bloch waves for a potential $V(x)$ that is specified in the interval between 0 and a . A discussion of the calculation can be found below the form.



Velocity of k -states



$$v = \frac{1}{\hbar} \frac{dE}{dk}$$

Student Projects

Calculate some transport property for a free electron gas or for a semiconductor.

Numerically calculate a transport property for a one dimensional material.