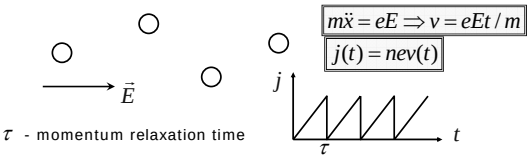
Boltzmann equation

- Drude-Sommerfeld model
- Distribution function
- Boltzmann equation
- Impurity scattering
- Conductivity
- Thermal conductivity
- Electron-electron scattering
- Umklapp processes

Drude-Sommerfeld model



$m\ddot{x} = eE \Rightarrow v = eEt/m$

$j(t) = nev(t)$

τ - momentum relaxation time

$j_{\max} = \sigma E$

$\sigma = ne^2\tau/m$ - serves as a reference point

Drude-Sommerfeld model

Problems with the Drude-Sommerfeld model:

- Is based on notions which are incorrect;
- Does not account for proper crystalline structure;
- Uses a phenomenological parameter;
- Does not account for inelastic scattering;
- It is not clear how other quantities could be calculated (*e.g.* thermal conductivity).

Distribution function

Electron as a wave packet: characterized by coordinate and momentum

Distribution function: $f(\vec{r},\vec{p},t)$

$f(\vec{r},\vec{p},t)d^3\vec{r}d^3\vec{p}$ - # of electrons in an element of the phase space

At equilibrium: Fermi function $f_F(\vec{p}) = \left[1+\exp(\varepsilon/k_BT)\right]^{-1}$ $\varepsilon = \varepsilon(\vec{p})$

Out of equilibrium: The system wants to relax to the Fermi function

External fields: distribution function depends on $\vec{r}$

Time-dependent external fields: distribution function depends on *t*

Relaxation to equilibrium is described by the Boltzmann equation.

Boltzmann equation

Nor specific to electrons in metals; a very general description of evolution

$df_i/dt = I[f]$

Left-hand side: time evolution of the distribution function of a certain state *i*

(time evolution of the number of particles in this state)

How can this number change?

Particles are transferred from this state to all other states and vice versa!

These particle transfers are described by the collision integral *I[f]* on the right-hand side

At equilibrium: no particle transfers between the states

Weak deviations from equilibrium: *I[f]* is a linear functional

The simplest form: $I[f_i] = -\gamma(f_i - f_F)$

Boltzmann equation

$df/dt = I[f]$

Left-hand side: $df/dt = \partial f/\partial t + \vec{v}\vec{\nabla}f + \dot{p}\partial f/\partial\vec{p}$

Time-dependent external fields (optical phenomena; sound attenuation)

Non-uniform external fields (thermopower, thermal conductivity)

External force (conductivity)

$\dot{p} = e\vec{E} + (e/c)\vec{v}\times\vec{B}$

Scattering probability

One electron scattered on an impurity: Born approximation

Probability of scattering from p to p': $w_{\vec{p}'\vec{p}} = \frac{2\pi}{\hbar}\left|V_{\vec{p}'\vec{p}}\right|^2 \delta(\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}'})$

V – matrix element of the impurity potential: $V(\vec{r}) = \sum_i v(\vec{r} - \vec{r}_i)$

$\vec{r}_i$ - impurity positions

Need to calculate the matrix element in Bloch functions. Result:

$V_{\vec{p}'\vec{p}} = \frac{1}{V}\sum_i e^{i(\vec{p}-\vec{p}')\vec{r}_i/\hbar} v_{\vec{p}'\vec{p}}$ $v_{\vec{p}'\vec{p}}$ - matrix element of v

Depends on impurity positions – too bad! Need to average over impurities.

Impurity averaging

$$\left\langle \left|V_{\vec{p}'\vec{p}}\right|^2 \right\rangle = \frac{1}{V^2}\left\langle \sum_{ik} e^{i(\vec{p}-\vec{p}')(\vec{r}_i-\vec{r}_k)} \right\rangle \left|v_{\vec{p}'\vec{p}}\right|^2$$

Terms with $i \neq k$: quickly oscillate ⟹ Average to zero.

Terms with $i=k$: give the number of impurities N_i

$\left\langle \left|V_{\vec{p}'\vec{p}}\right|^2 \right\rangle = \frac{n_i}{V}\left|v_{\vec{p}'\vec{p}}\right|^2$ $n_i \equiv \frac{N_i}{V}$ - impurity concentration

$$w_{\vec{p}'\vec{p}} = \frac{2\pi n_i}{\hbar V}\left|v_{\vec{p}'\vec{p}}\right|^2 \delta(\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}'})$$

Collision integral

$df_{\vec{p}}/dt = I[f]$ $I[f_{\vec{p}}] = 2_s V \int \frac{d^3\vec{p}'}{(2\pi\hbar)^3}\left[-w_{\vec{p}'\vec{p}} f_{\vec{p}}(1-f_{\vec{p}'}) + w_{\vec{p}\vec{p}'} f_{\vec{p}'}(1-f_{\vec{p}})\right]$

Scattering out: Loss of particles

Scattering in: Gain of particles

Equilibrium function: only depends on energy; $I[f_{eq}] = 0$

To simplify: isotropic model: $w_{\vec{p}\vec{p}'}$ only depends on p-p'

$I[f] = -(f - f_{eq})/\tau$

Relaxation (transport) time: $\tau^{-1} = \frac{\pi n_i \nu}{\hbar}\int \frac{d\Omega}{4\pi}\left|v(\theta)\right|^2 (1-\cos\theta)$

Conductivity

External electric field $\vec{E} \,||\, \hat{z}$, assume relaxation time approximation

Need to
- solve the kinetic equation and find the distribution function;
- calculate the current as the function of the field.

Field is time- and position independent ⟹ f only depends on p.

$e\vec{E}\partial f/\partial\vec{p} = I[f] = -(f - f_{eq})/\tau$

Solution:

Expansion in powers of the electric field $f = f_{eq}(\varepsilon) + f_1(\vec{p})$ $f_1(\vec{p}) \propto \vec{E}$

$e\vec{E}\partial f_{eq}/\partial\vec{p} = -f_1(\vec{p})/\tau$

Conductivity

$f_1(\vec{p}) = -e\vec{E}\tau\partial f_{eq}/\partial\vec{p}$

Note that $\partial f_{eq}/\partial\vec{p} = (df_{eq}/d\varepsilon)\cdot(\partial\varepsilon/\partial\vec{p}) = \vec{v} f'_{eq}$

$f_1 = -e\vec{E}\vec{v}\tau df_{eq}/d\varepsilon$

Current density: $\vec{j} = 2_s e\int \vec{v} f \frac{d^3\vec{p}}{(2\pi\hbar)^3}$ Contribution of f_{eq} - zero (equilibrium current)

$\vec{j} = -e^2\int d\varepsilon \frac{d\Omega}{4\pi} g(\varepsilon)\vec{v}(\vec{v}\cdot\vec{E})\tau\frac{df_{eq}}{d\varepsilon} \approx \frac{1}{3}e^2\vec{E}\left(g v^2\tau\right)_{\varepsilon=\mu}$

$\vec{j} = \sigma\vec{E}$ $\sigma = \frac{1}{3}e^2\left(g v^2\tau\right)_{\varepsilon=\mu}$

Conductivity

$\sigma = \frac{1}{3}e^2\left(g v^2\tau\right)_{\varepsilon=\mu}$

Let us compare with the Drude-Sommerfeld formula for the free electron gas $\sigma = ne^2\tau/m$

Electron density: $n_e(\mu) = \frac{1}{3\pi^2\hbar^3}(2m\mu)^{3/2}$ Density of states: $g(\mu) = \frac{\sqrt{2}}{\pi^2\hbar^3} m^{3/2}\sqrt{\mu}$ Ok!

Estimates for Cu: (Lecture 2) $c_i \sim 10^{-5} \Rightarrow l \sim 10\mu m$; $v_F \approx 10^6 m/s$

$\tau \sim 10^{-11} s = 10 ps$

$\sigma \approx 10^{-10}(\Omega\cdot m)^{-1}$

Thermal conductivity

Uniform temperature gratient dT/dz, assume relaxation time approximation

This is not a force!

$$\vec{v}\vec{\nabla}f = v_z \frac{\partial f}{\partial T}\frac{\partial T}{\partial z} = -(f - f_{eq})/\tau$$

Solution:

Expansion in powers of the temperature gradient

$$f = f_{eq}(\varepsilon) + f_1(\vec{p}) \qquad f_1(\vec{p}) \propto \vec{\nabla}T$$

$$\Downarrow$$

$$v_z \frac{\partial T}{\partial z}\frac{\partial f}{\partial T} = -f_1(\vec{p})/\tau$$

Thermal conductivity

$$v_z \frac{\partial T}{\partial z}\frac{\partial f_{eq}}{\partial T} = -f_1(\vec{p})/\tau$$

Note that $\partial f_{eq}/\partial T = -(\varepsilon - \mu) f'_{eq}/T$ ➡ $$f_1 = v_z \frac{\partial T}{\partial z}\tau \frac{\varepsilon - \mu}{T}\frac{df_{eq}}{d\varepsilon}$$

Heat current density: $$\vec{q} = 2_s e\int \vec{v}(\varepsilon - \mu) f \frac{d^3\vec{p}}{(2\pi\hbar)^3}$$ Contribution of f_{eq} - zero

$$\vec{q} = -\frac{\pi^2}{9}k_B^2 T \frac{\partial T}{\partial z}\left(g v^2 \tau\right)_{\varepsilon=\mu} \qquad \kappa = \frac{\pi^2 k_B^2 T}{9}\left(g v^2 \tau\right)_{\varepsilon=\mu}$$

$$\vec{q} = -\kappa\vec{\nabla}T$$

Wiedemann-Franz law

$$\kappa = \frac{\pi^2 k_B^2 T}{9}\left(g v^2 \tau\right)_{\varepsilon=\mu} \qquad \sigma = \frac{1}{3}e^2\left(g v^2 \tau\right)_{\varepsilon=\mu}$$

$$\frac{\kappa}{\sigma T} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2$$ - Wiedemann-Franz law

Conditions:
- Elastic scattering;
- Isotropic scattering

Collision integral for electron-electron scattering

$$I[f_{\vec{p}_1}] = (2_s V)^3 \int \frac{d^3\vec{p}_2 d^3\vec{p}\,'_1 d^3\vec{p}\,'_2}{(2\pi\hbar)^9} \times \left[-w_{\vec{p}'_1\vec{p}'_2;\vec{p}_1\vec{p}_2} f_{\vec{p}_1} f_{\vec{p}_2}(1 - f_{\vec{p}_1})(1 - f_{\vec{p}'_2}) + w_{\vec{p}_1\vec{p}_2;\vec{p}'_1\vec{p}'_2} f_{\vec{p}'_1} f_{\vec{p}'_2}(1 - f_{\vec{p}_1})(1 - f_{\vec{p}_2})\right]$$

Scattering out: Loss of particles

Scattering in: Gain of particles

Functions *w* take care of the energy and momentum conservation and contain matrix element of electron-electron interaction

Under certain conditions, *I[f]* can be written in the relaxation time approximation

$$I[f] = -(f - f_{eq})/\tau_\varepsilon$$ τ_ε - energy relaxation time

Conductivity

$I[f] = -(f - f_{eq})/\tau_\varepsilon$ $\hbar/\tau_\varepsilon \propto \varepsilon^2$ - phase space consideratons

The only possible combination: $\hbar/\tau_\varepsilon \sim \varepsilon^2/\mu$

Conductivity:

$$\sigma \sim e^2 g v_F^2 \tau_\varepsilon \sim \hbar g v_F^3 \mu/\hbar(k_B T)^2 \sim (\mu/k_B T)^2 (p_F^2/\hbar m)$$

Is only important in **very** clean metals at low temperatures:

At low temperatures, impurities are important;
At higher temperatures, phonons determine the conductivity.

Umklapp processes

A problem: the total electron momentum is conserved in electron-electron collisions. But dissipation means electron stream slows down. How could this happen?

There are processes that do not conserve the momentum!

$$\vec{p}_1 + \vec{p}_2 = \vec{p}\,'_1 + \vec{p}\,'_2$$

$$\Downarrow$$

$$\vec{p}_1 + \vec{p}_2 - \vec{p}\,'_1 - \vec{p}\,'_2 = \hbar\vec{K}$$

For $\vec{K} \neq 0$ - Umklapp processes – do not conserve the total momentum of the electron system

Umklapp processes

$$\vec{p}_1 + \vec{p}_2 - \vec{p}\,'_1 - \vec{p}\,'_2 = \hbar\vec{K}$$

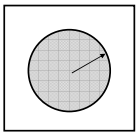
What are the conditions under which Umklapp processes are possible?

$$4p_{\max} \geq \hbar K_{\min}$$

Example: alkali metals
One electron per atom

$$p_F = \hbar\left(3\pi^2 N/V\right)^{1/3}$$

$$N/V = 1/a^3$$



$$K_{\min} = 2\pi/a$$

$$p_F = (\hbar/a)(3\pi^2)^{1/3}$$
$$= \hbar K_{min}(3/8\pi)^{1/3}$$
$$> \hbar K_{min}/4$$

Umklapp processes possible!