The Boltzmann Transport Equation

To the extent that electrons can be considered as particles

The Boltzmann transport equation is a statement that in the steady state, there is no net change in the distribution function $f(\mathbf{r}, \mathbf{k}, t)$ which determines the probability of finding an electron at position $\mathbf{r}$, with crystal momentum $\mathbf{k}$ and at time t.

we obtain a zero sum for the changes in $f(\mathbf{r}, \mathbf{k}, t)$ due to the 3 processes of diffusion, the effect of forces and fields, and of collisions:

$$\left.\frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t}\right|_{\text{diffusion}} + \left.\frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t}\right|_{\text{fields}} + \left.\frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t}\right|_{\text{collisions}} = 0.$$

It is customary to substitute the following differential form for the diffusion process

$$\left.\frac{\partial f(\mathbf{r},\mathbf{k},t)}{\partial t}\right|_{\text{diffusion}} = -\mathbf{v}(\mathbf{k})\cdot\frac{\partial f(\mathbf{r},\mathbf{k},t)}{\partial \mathbf{r}}$$

which expresses the continuity equation in real space in the absence of forces, fields and collisions. For the forces and fields, we write correspondingly

$$\left.\frac{\partial f(\mathbf{r},\mathbf{k},t)}{\partial t}\right|_{\text{fields}} = -\frac{\partial \mathbf{k}}{\partial t}\cdot\frac{\partial f(\mathbf{r},\mathbf{k},t)}{\partial \mathbf{k}}$$

$$\left.\frac{\partial f}{\partial t}\right|_{\substack{\text{explicit}\\ \text{time}\\ \text{dependence}}} + \vec{v}(\vec{k})\cdot\frac{\partial f}{\partial \vec{r}} + \frac{\partial \vec{k}}{\partial t}\cdot\frac{\partial f}{\partial \vec{k}} = \left.\frac{\partial f}{\partial t}\right|_{\text{collisions}}$$

$\rightarrow$ Eq. (1)

First approximation

The perturbation due to external fields and forces is assumed to be small so that the distribution function can be linearized and written as —

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

$f_0(E)$ is the equilibrium distribution function (the Fermi function) which depends only on energy E.

$f_1(\vec{r},\vec{k})$ is the perturbation term giving the departure from equilibrium.

Second approximation

- The collision term in the Boltzmann equation is written in the relaxation time approximation so that the system returns to equilibrium uniformly.

$$\left.\frac{\partial f}{\partial t}\right|_{collisions} = (-)\frac{(f-f_0)}{\tau} = (-)\frac{f_1}{\tau}$$

'τ' is the relaxation time and is a function of crystal momentum, i.e. $\tau = \tau(\vec{K})$

- The physical interpretation of the relaxation time is the time associated with the rate of return to the equilibrium distribution when the external fields or thermal gradients are switched off.

When the fields are switched off at $t=0$

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

$$f(t) = f_0 + [f(0) - f_0]e^{-t/\tau}$$

f_0 is the equilibrium distribution (Fermi) function and $f(0)$ is the distribution function at $t=0$ sec.

Solution of The Boltzmann Transport Equation

The current density $\mathbf{j}(\mathbf{r}, t)$ is given by

$$\mathbf{j}(\mathbf{r}, t) = \frac{e}{4\pi^3} \int \mathbf{v}(\mathbf{k}) f(\mathbf{r}, \mathbf{k}, t) d^3k$$

average of $\langle ne\vec{v} \rangle$ over all k-space

in which the crystal momentum $\hbar\mathbf{k}$ plays the role of the momentum $\mathbf{p}$ in specifying a volume in phase space d^3k. Every element of size h (Planck's constant) in phase space can accommodate one spin ↑ and one spin ↓ electron. The carrier density $n(\mathbf{r}, t)$ is thus simply given by integration of the distribution function over k-space

$$n(\mathbf{r}, t) = \frac{1}{4\pi^3} \int f(\mathbf{r}, \mathbf{k}, t) d^3k$$

In d^3k, there are $\left(\overset{\text{for two spins}}{2} \times V \frac{d^3k}{(2\pi)^3} \right)$ no. of 'k' states

The velocity of a carrier with crystal momentum $\hbar\vec{K}$ is related to the $E(\vec{K})$ dispersion

$$\vec{v}(\vec{K}) = \frac{1}{\hbar}\frac{\partial E(\vec{K})}{\partial \vec{K}}$$

$$f_0(E) = \frac{1}{e^{(E-E_F)/KT}+1}$$

$E_F \rightarrow$ Fermi energy

$$f(t) = f_0 + \left[f(0) - f_0\right]e^{-t/\tau}$$

Electrical Conductivity

Static electrical conductivity in presence of an applied electric field $\vec{E}$ applied along x- direction. No thermal gradients are present

The electrical conductivity is expressed in terms of the conductivity tensor $\overleftrightarrow{\sigma}$

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

$$\left.\frac{\partial f}{\partial t}\right|_{\substack{\text{explicit}\\ \text{time}\\ \text{dependence}}} + \vec{v}(\vec{k})\cdot\frac{\partial f}{\partial \vec{r}} + \frac{\partial \vec{k}}{\partial t}\cdot\frac{\partial f}{\partial \vec{k}} = \left.\frac{\partial f}{\partial t}\right|_{\text{collisions}}$$

$\rightarrow$ Eq. 1

Since dc applied field has no time dependence, first term in Eq 1 vanishes.

$$\underbrace{\frac{\partial f}{\partial \vec{r}} \simeq \frac{\partial f_0}{\partial \vec{r}}} = \frac{\partial f_0}{\partial T}\frac{\partial T}{\partial \vec{r}} = 0 \quad \left[\begin{array}{l}\text{No thermal gradients}\\ \text{are present}\end{array}\right]$$

Since f_1 is already due to perturbation. In linearized Boltzmann equation, we retain only leading order terms in the perturbation.

$$\dot{\vec{k}} \cdot \frac{\partial f(\vec{r},\vec{k},t)}{\partial \vec{k}} = \sum_{\alpha} \dot{k}_{\alpha} \frac{\partial f(\vec{r},\vec{k},t)}{\partial k_{\alpha}}$$

Also, $\hbar \dot{\vec{k}} = e\vec{E}$

$$\frac{\partial f}{\partial \vec{k}} = \frac{\partial (f_0 + f_1)}{\partial \vec{k}} = \frac{\partial f_0}{\partial E}\frac{\partial E}{\partial \vec{k}} + \underbrace{\frac{\partial f_1}{\partial \vec{k}}}$$

Not considering this since only terms linear in perturbing electric field are to be considered.

$$\dot{\vec{k}} \cdot \frac{\partial f}{\partial \vec{k}} = \dot{\vec{k}} \cdot \frac{\partial f_0}{\partial E} \frac{\partial E}{\partial \vec{k}}$$

$$= \frac{e\vec{E}}{\hbar} \cdot \frac{\partial f_0}{\partial E} \frac{\partial E}{\partial \vec{k}}$$

$$= \frac{e\vec{E}}{\hbar} \cdot \frac{\partial f_0}{\partial E} \hbar \vec{v}(\vec{k}) \qquad \left[\because \vec{v} = \frac{1}{\hbar} \frac{\partial E}{\partial \vec{k}}\right]$$

Also,

$$\vec{j} = \frac{1}{4\pi^3}\int e\vec{v}(\vec{k})\, f(\vec{k})\, d^3k$$

$$= \frac{1}{4\pi^3}\int e\vec{v}(\vec{k})\left[f_0(\vec{k}) + f_1(\vec{k})\right] d^3k \rightarrow (2)$$

Since no net current flows in absence of applied electric field

$$\int e\vec{v}(\vec{k})\, f_0(\vec{k})\, d^3k = 0$$

From Boltzmann equation (1) —

$$\frac{e\vec{E}}{\hbar} \cdot \frac{\partial f_0}{\partial E} \hbar \vec{v}(\vec{k}) = (-) \frac{f_1}{\tau}$$

$$\longrightarrow \quad \vec{j} = (-) \frac{e^2 \vec{E}}{4\pi^3} \int \vec{v}\,\vec{v} \left(\frac{\partial f_0}{\partial E}\right) \tau\, d^3K$$

depends on $E(\vec{k})$ relation

Captures temp. dependence

$$\overleftrightarrow{\sigma} = (-) \frac{e^2}{4\pi^3} \int \tau\, \vec{v}\,\vec{v} \left(\frac{\partial f_0}{\partial E}\right) d^3K .$$

$\overleftrightarrow{\sigma}$ is a symmetric second-rank tensor $(\sigma_{ij} = \sigma_{ji})$

Electrical Conductivity in Metals

Let us replace $\int d^3K$ with an integral over the constant energy surfaces —

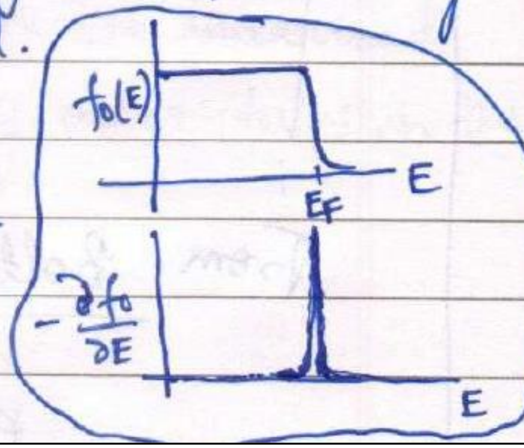
$$\int d^3k = \int d^2S\, dk_\perp = \int d^2S \frac{dE}{\left|\frac{\partial E}{\partial \vec{k}}\right|}$$

$$\overleftrightarrow{\sigma} = (-)\frac{e^2}{4\pi^3} \int \frac{\tau \vec{v} \vec{v}}{\left|\frac{\partial E}{\partial \vec{k}}\right|} \frac{\partial f_0}{\partial E}\, d^2S\, dE$$

$f_0(E) \rightarrow$ Fermi-Dirac distribution function

The derivative can approximately be replaced by a delta function for the case of a metal.

$$\overleftrightarrow{\sigma} = \frac{e^2}{4\pi^3\hbar} \int_{\substack{\text{Fermi}\\ \text{surface}}} \tau \vec{v} \vec{v} \frac{d^2 s}{v}$$



For a cubic crystal, $\overleftrightarrow{\sigma}$ has only diagonal components σ which are all equal.

$$\sigma = \frac{e^2}{4\pi^3\hbar} \int_{\substack{\text{Fermi}\\ \text{Surface}}} \tau v \frac{d^2 s}{3}$$

$$\because \left(v_x^2 = \frac{v^2}{3} = v_y^2 = v_z^2 \right)$$

Electrical conducitivity in Metals

$$\sigma = \frac{e^2}{4\pi^3\hbar} \frac{\tau v_F}{3} 4\pi k_F^2$$

$k_F \rightarrow$ Fermi wavevector

$v_F \rightarrow$ Fermi velocity

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

$$\left[\text{as, } v_F = \frac{\hbar k_F}{m^*} \quad \text{and} \quad n = \frac{1}{4\pi^3} \frac{4}{3}\pi k_F^3 = \frac{1}{3\pi^2} k_F^3 \right]$$

m* is the effective mass of electrons depending on band structure