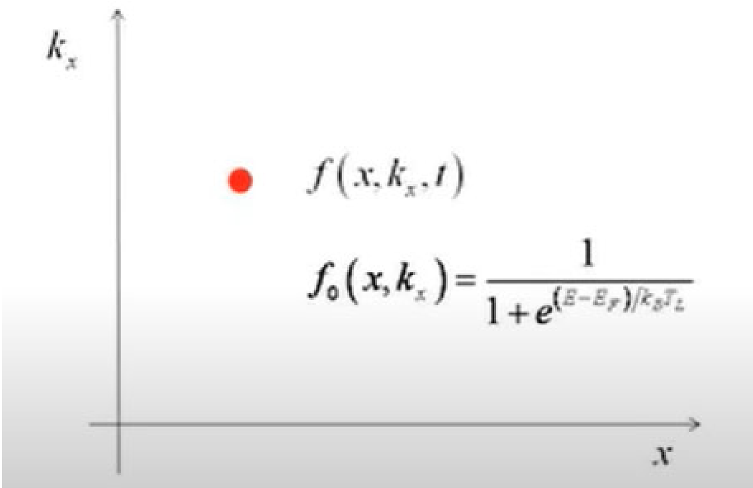
Boltzmann Transport equation

Boltzmann Transport equation (BTE) is very useful in understanding the transport properties such as electrical conductivity, thermal conductivity, and thermoelectric power.

This equation is used to determine the distribution function of particles (electrons) in the phase space (***r***, ***k***).



Consider simply a particle present in a simple 1D space (in phase space 1D has two coordinates x and p_x). The probability of a particle occupying a particular state at equilibrium condition can be expressed through Fermi function.

Question is how this probability or distribution function looks like in 3D space and how it affects with collision or force of the electrons?

BTE is a semi-classical equation considering electron as semi-classical particle which obeys following modified Newtons equations.

$$\frac{d(\hbar\vec{k})}{dt} = -\nabla_r E_C(r) = -q\vec{\xi}(\vec{r})$$

$$\hbar\vec{k}(t) = \hbar\vec{k}(0) + \int_0^t -q\vec{\xi}(t')\,dt'$$

$$\vec{v}_g(t) = \frac{1}{\hbar}\nabla_k E\left[\vec{k}(t)\right]$$

$$\vec{r}(t) = \vec{r}(0) + \int_0^t \vec{v}_g(t')dt'$$

$\hbar\vec{k}$ - momentum

E_C - conduction band bottom energy

$\vec{\xi}(\vec{r})$ - Electric field

Consider the electron present in a energy band described by Bloch function $\psi_k(\vec{r}) = |\vec{k}\rangle = e^{ik.r}u_k(\vec{r})$

The number of electrons per unit volume whose wavevectors lie in the interval (***k*** - ***k***+d***k***) is

$$\frac{2}{(2\pi)^3} f(\vec{k}, \vec{r}) d\vec{k}$$

where the factor 2 is the spin weight. In equilibrium $f(\boldsymbol{k}, \boldsymbol{r})$ becomes the Fermi-Dirac distribution function $f_0(E)$, but deviates from $f_0(E)$ in the presence of the electric field, magnetic field, temperature gradient, and so on. There are two contributions this time dependence, (i) from the external force (the drift term) and (ii) the collisions (the collision term),

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t}\right)_{drift} + \left(\frac{\partial f}{\partial t}\right)_{coll}$$

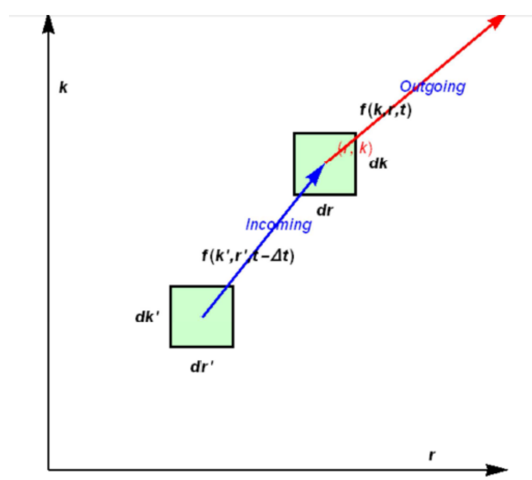
If we consider the evolution of a particle as in this graph, the function in the dimension drdk is f(k,r,t) and the same function is f(k', r', t - Δt) in dr'dk'.

If there is no collision only external force is applied, then

$$f(\vec{k}, \vec{r}, t) = f(\vec{k}', \vec{r}' t - \Delta t)$$

$$\frac{\partial f}{\partial t} = 0$$

Its called as Collison less BTE – Ballistic transport



The above equation can be written as

$$\frac{\partial f}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_{drift} + \frac{\partial f}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial f}{\partial p_x}\frac{\partial p_x}{\partial t} = 0$$

$$\frac{\partial f}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_{drift} + \frac{\partial f}{\partial x}v_x + \frac{\partial f}{\partial p_x}F_x = 0$$

For three dimensions,

$$\left(\frac{\partial f}{\partial t}\right)_{drift} + \vec{v}\nabla_r f + \vec{F_e}.\nabla_p f = 0$$

$$\left(\frac{\partial f}{\partial t}\right)_{drift} = \overrightarrow{-v}\nabla_r f - \vec{F_e}.\nabla_p f = 0$$

$$\vec{F_e} = -q\vec{E} - q\vec{\upsilon}\times\vec{B}$$

$$\nabla_r f = \frac{\partial f}{\partial x}\hat{x} + \frac{\partial f}{\partial y}\hat{y} + \frac{\partial f}{\partial z}\hat{z}$$

$$\nabla_p f = \frac{\partial f}{\partial p_x}\hat{p}_x + \frac{\partial f}{\partial p_y}\hat{p}_y + \frac{\partial f}{\partial p_z}\hat{p}_z$$

$$\vec{p} = \hbar\vec{k}$$

Assumptions considered in above collision less BTE

1. Semiclassical treatment of electrons in a crystal with E(k)
2. Neglected generation and recombination
3. Neglected e-e correlations (mean field approximation)

Whereas, the collision term can be written as

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = -\frac{f - f_0(\boldsymbol{k})}{\tau(\boldsymbol{k})},$$

Where f_0 – equilibrium distribution function
f – distribution function after a collision
τ – relaxation time

We consider the general Boltzmann equation

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t}\right)_{drift} + \left(\frac{\partial f}{\partial t}\right)_{colli}$$

In the steady state, $\frac{df}{dt} = 0$

$$\left(\frac{\partial f}{\partial t}\right)_{drift} + \left(\frac{\partial f}{\partial t}\right)_{colli} = 0$$

$$f = f_0 - \tau\vec{v}.\nabla_r f - \frac{1}{\hbar}\tau\vec{F}\nabla_k f$$

$$\vec{F}_e = -q\vec{E} - q\vec{\upsilon}\times\vec{B}$$

$$\nabla_r f = \frac{\partial f}{\partial x}\hat{x} + \frac{\partial f}{\partial y}\hat{y} + \frac{\partial f}{\partial z}\hat{z}$$

$$\nabla_p f = \frac{\partial f}{\partial p_x}\hat{p}_x + \frac{\partial f}{\partial p_y}\hat{p}_y + \frac{\partial f}{\partial p_z}\hat{p}_z$$

$$\vec{p} = \hbar\vec{k}$$

$$-v.\nabla_r f - \frac{1}{\hbar}F.\nabla_k f - \frac{(f - f_0(k))}{\tau_k} = 0$$

$$-v.\tau.\nabla_r f - \frac{1}{\hbar}F.\tau.\nabla_k f + f_0(k) = f$$

$$\boxed{f = f_0(k) - v.\tau.\nabla_r f - \frac{1}{\hbar}F.\tau.\nabla_k f}$$

This equation is called the Boltzmann equation.