Chapter 4

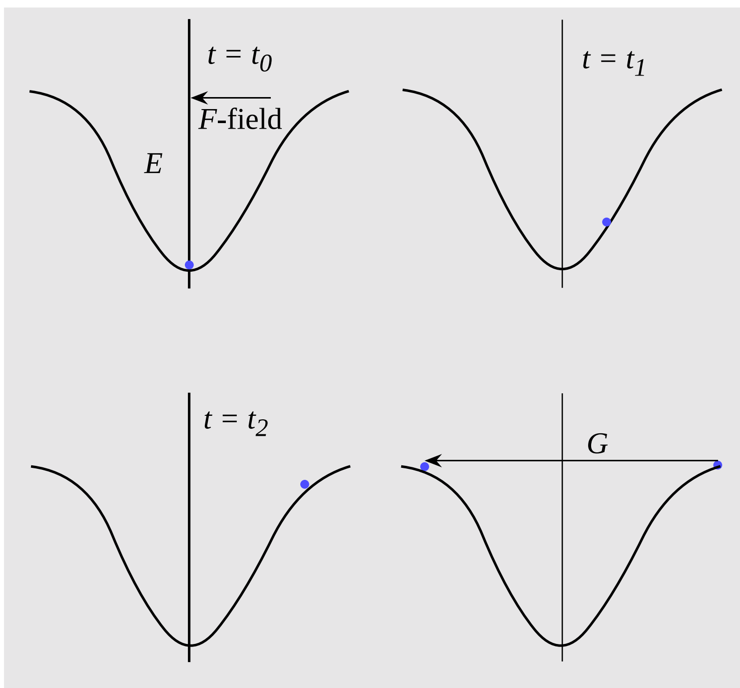
TRANSPORT: GENERAL FORMALISM

TRANSPORT AND SCATTERING OF CARRIERS

In a perfectly periodic material, electrons suffer no scattering and obey the equation

$$\hbar \frac{dk}{dt} = \text{Force}$$

If an electric field is applied the electrons will oscillate in *k*-space—from the *k*=0 to zone edge *k*-value, as shown. Such oscillations are called *Bloch Zener oscillations* and can, in principle, generate terrahertz radiation. However, in real semiconductors scattering occurs and destroys the possibility of these oscillations.



The motion of an electron in a band in the absence of any scattering and in the presence of an electric field. The electron oscillates in *k*-space gaining and losing energy from the field.

© Prof. Jasprit Singh www.eecs.umich.edu/~singh

SCATTERING OF ELECTRONS

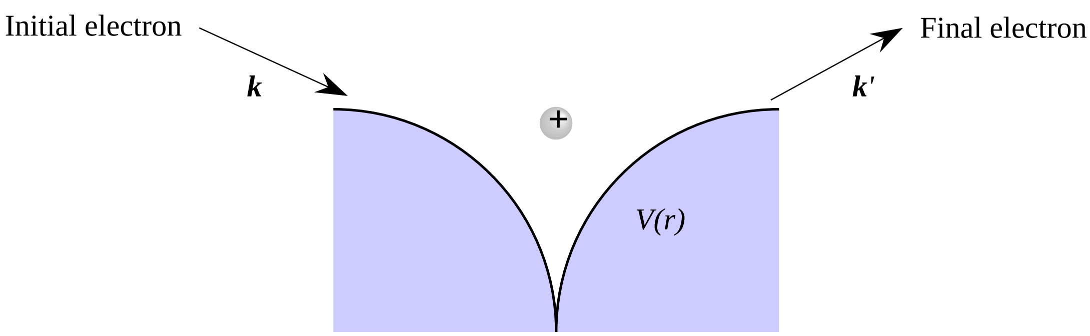
In semiconductor physics scattering is described by first (or if necessary, second) order perturbation theory.

Full problem: $H = H_0 + V$

Simple problem: $H_0 \psi_k = E\psi_k$ → The periodic structure

Perturbation: V → Source of scattering

The perturbation causes scattering of electrons from a state $\boldsymbol{k}$ to $\boldsymbol{k}'$. The scattering rate is given (in first order) by the Fermi Golden Rule:



Scattering potential

Scattering rate	α	How strongly $V(r)$ couples the initial and final states.
	α	How many final states there are to scatter into.

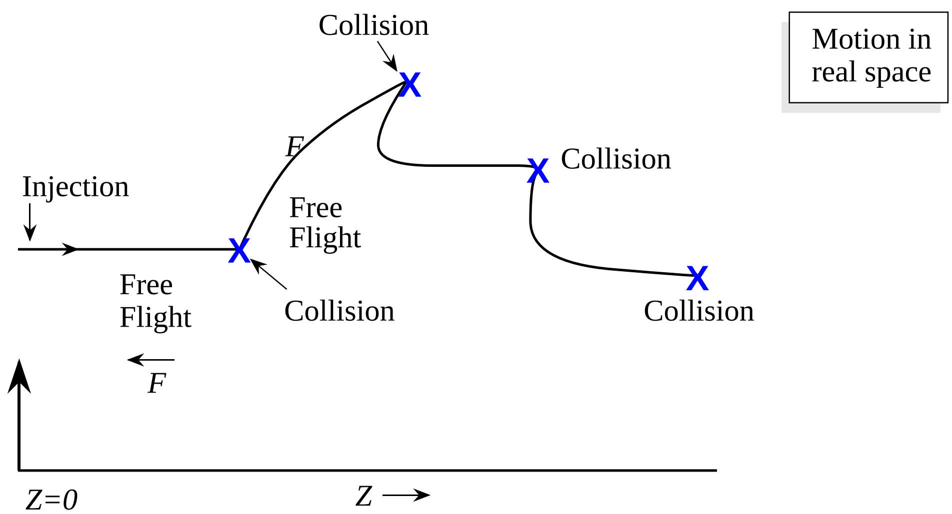
$$V(r,t) = V(r) \exp(i\omega t)$$

Scattering rate: $$W_{if} = \frac{2\pi}{\hbar} \left| M_{ij} \right|^2 \delta(E_i \pm \hbar\omega - E_f)$$

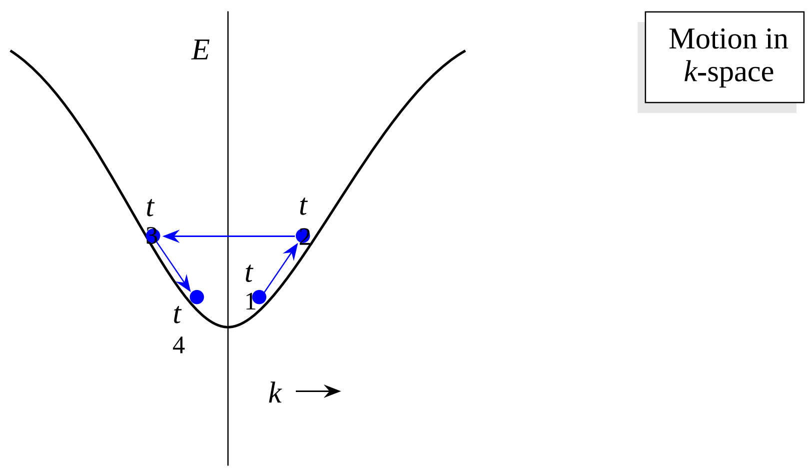
Matrix element: $$M_{ij} = \quad \psi_f^* V(r) \psi_i d^3 r$$

© Prof. Jasprit Singh www.eecs.umich.edu/~singh

TRANSPORT IN THE PRESENCE OF SCATTERING: A PHYSICAL VIEW



A schematic view of an electron as it moves under an electric field in a semiconductor. The electron suffers a scattering as it moves. In between scattering the electron moves according to the “free” electron equation of motion.



In the presence of scattering the electron moves in the band in a random manner. The presence of an electric field produces a net drift.

© Prof. Jasprit Singh www.eecs.umich.edu/~singh

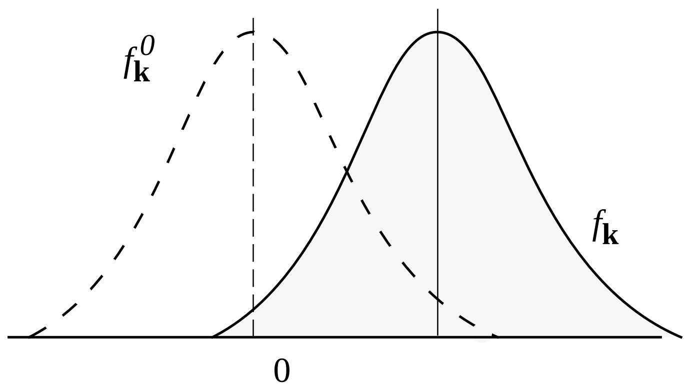
Scattering theory: distribution function

In scattering theory we are trying to find the distribution function for the carriers in the presence of external perturbations (electric field, magnetic field, etc.).

$f^0_{\mathbf{k}}(E) \Rightarrow$ equilibrium distribution function

$$= \frac{1}{\exp\left(\frac{E-E_F}{k_BT}\right)+1}$$

$f_{\mathbf{k}}(E) \Rightarrow$ non-equilibrium distribution function = ?



The displaced distribution function shows the effect of an applied electric field.

Macroscopic physical parameters: drift velocity
average energy
.
.
.

$$\langle A \rangle = \frac{\int f_{\mathbf{k}}(E)\, A\, \frac{d^3k}{(2\pi)^3}}{\int f_{\mathbf{k}}(E)\, \frac{d^3k}{(2\pi)^3}}$$

© Prof. Jasprit Singh www.eecs.umich.edu/~singh

TRANSPORT THEORY: TWO APPROACHES

How do we obtain the non-equilibrium distribution function?

• BOLTZMANN TRANSPORT THEORY:

Distribution function changes due to:
- Diffusion of carriers
- External forces
- Scattering

Write a balance equation for these changes $\Longrightarrow$ Transport equation

Boltzmann transport equation (BTE) can be solved numerically to obtain $f_{\mathbf{k}}(E)$

• MONTE CARLO METHOD:

This is a computer simulation method where electrons are followed in real space, momentum space, and energy space as they move through a material. Scattering processes are simulated by the use of random numbers. By keeping track of the electrons' properties we can obtain macroscopic properties of the electron gas.

© Prof. Jasprit Singh www.eecs.umich.edu/~singh

BOLTZMANN TRANSPORT EQUATION

Distribution function $f_{\mathbf{k}}(E)$ can change due to three reasons:

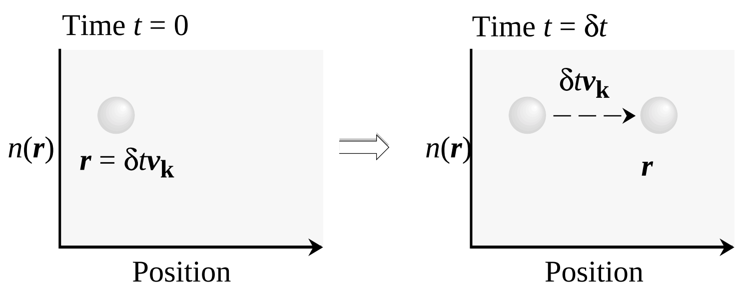
1. Due to the motion of the electrons (diffusion), carriers will be moving into and out of any volume element around $\boldsymbol{r}$.

2. Due to the influence of external forces, electrons will be changing their momentum (or $\boldsymbol{k}$-value) according to $\hbar\, d\boldsymbol{k}/dt = \boldsymbol{F}_{ext}$.

3. Due to scattering processes, electrons will move from one $\boldsymbol{k}$-state to another.

DIFFUSION-INDUCED EVOLUTION OF $f_{\mathbf{k}}(\boldsymbol{r})$

At time $t = 0$ particles at position $\boldsymbol{r} - \delta t \boldsymbol{v}_{\mathbf{k}}$ reach the position $\boldsymbol{r}$ at a later time δt. This simple concept is important in establishing the Boltzmann transport equation.



$$f_{\mathbf{k}}(\boldsymbol{r},\delta t) = f_{\mathbf{k}}(\boldsymbol{r} - \delta t\, \boldsymbol{v}_{\mathbf{k}},0)$$

or

$$f_{\mathbf{k}}(\boldsymbol{r},0) + \frac{f_{\mathbf{k}}}{t} \bullet \delta t = f_{\mathbf{k}}(\boldsymbol{r},0) - \frac{f_{\mathbf{k}}}{\boldsymbol{r}} \bullet \delta t\, \boldsymbol{v}_{\mathbf{k}}$$

$$\left.\frac{f_{\mathbf{k}}}{t}\right|_{\text{diff}} = -\frac{f_{\mathbf{k}}}{\boldsymbol{r}} \bullet \boldsymbol{v}_{\mathbf{k}}$$

EXTERNAL FIELD-INDUCED EVOLUTION OF $f_{\mathbf{k}}(\boldsymbol{r})$ $\qquad \dot{\boldsymbol{k}} = \frac{e}{\hbar}\,[\boldsymbol{E} + \boldsymbol{v}_{\mathbf{k}} \times \boldsymbol{B}]$

$$f_{\mathbf{k}}(\boldsymbol{r},\delta t) = f_{\mathbf{k}-\dot{\mathbf{k}}\delta t}(\boldsymbol{r},0)$$

which leads to the equation

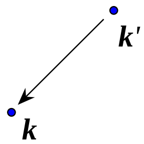
$$\left.\frac{f_{\mathbf{k}}}{t}\right|_{\text{ext.forces}} = -\dot{\boldsymbol{k}}\,\frac{f_{\mathbf{k}}}{\boldsymbol{k}}$$

$$= \frac{-e}{\hbar}\left[\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}\right] \bullet \frac{f_{\mathbf{k}}}{\boldsymbol{k}}$$

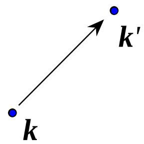
© Prof. Jasprit Singh www.eecs.umich.edu/~singh

BOLTZMANN TRANSPORT EQUATION

SCATTERING-INDUCED EVOLUTION OF $f_{\mathbf{k}}(\boldsymbol{r})$



$W(\boldsymbol{k}',\boldsymbol{k})$: rate of scattering into state $\boldsymbol{k}$



$W(\boldsymbol{k},\boldsymbol{k}')$: rate of scattering out of $\boldsymbol{k}$ into $\boldsymbol{k}'$

$$\left.\frac{f_{\mathbf{k}}}{t}\right)_{\text{scattering}} = \int \left[f_{\mathbf{k}'}(1 - f_{\mathbf{k}})\, W(\boldsymbol{k}',\boldsymbol{k}) - f_{\mathbf{k}}(1 - f_{\mathbf{k}'})\, W(\boldsymbol{k},\boldsymbol{k}') \right] \frac{d^3k'}{(2\pi)^3}$$

In steady state:

$$\left.\frac{f_{\mathbf{k}}}{t}\right)_{\text{scattering}} + \left.\frac{f_{\mathbf{k}}}{t}\right)_{\text{fields}} + \left.\frac{f_{\mathbf{k}}}{t}\right)_{\text{diffusion}} = 0$$

Let us define

$$g_{\mathbf{k}} = f_{\mathbf{k}} - f_{\mathbf{k}}^0$$

where $f_{\mathbf{k}}^0$ is the equilibrium distribution.

Substituting $f_{\mathbf{k}} = f_{\mathbf{k}}^0 + g_{\mathbf{k}}$

$$-\boldsymbol{v}_{\mathbf{k}} \cdot \nabla_r f_{\mathbf{k}}^0 - \frac{e}{\hbar} (\boldsymbol{E} + \boldsymbol{v}_{\mathbf{k}} \times \boldsymbol{B}) \nabla_k f_{\mathbf{k}}^0$$

$$= -\left.\frac{f_{\mathbf{k}}}{t}\right)_{\text{scattering}} + \boldsymbol{v}_{\mathbf{k}} \cdot \nabla_r g_{\mathbf{k}} + \frac{e}{\hbar} (\boldsymbol{E} + \boldsymbol{v}_{\mathbf{k}} \times \boldsymbol{B}) \cdot \nabla_k g_{\mathbf{k}}$$

Evaluating the derivatives of $f_{\mathbf{k}}^0$ we get

$$-\frac{f^0}{E_{\mathbf{k}}} \cdot \boldsymbol{v}_{\mathbf{k}} \cdot \left[-\frac{(E_{\mathbf{k}} - \mu)}{T} \nabla \boldsymbol{T} + e\boldsymbol{E} - \nabla\mu \right]$$

$$= -\left.\frac{f}{t}\right)_{\text{scattering}} + \boldsymbol{v}_{\mathbf{k}} \cdot \nabla_r g_{\mathbf{k}} + \frac{e}{\hbar} (\boldsymbol{v}_{\mathbf{k}} \times \boldsymbol{B}) \cdot \nabla_k g_{\mathbf{k}}$$

© Prof. Jasprit Singh www.eecs.umich.edu/~singh

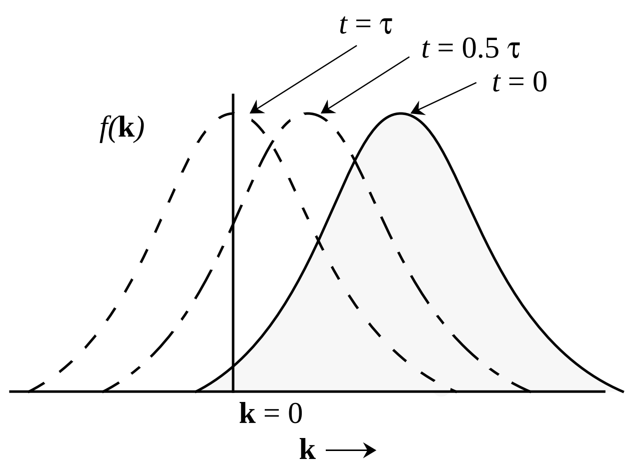
BOLTZMANN TRANSPORT EQUATION: AN APPROXIMATE TREATMENT

ASSUMPTIONS: Electric field is small, uniform
Magnetic field is zero
No temperature variations in space

$$\Rightarrow \quad - \frac{f^0}{E_k} \boldsymbol{v}_{\mathbf{k}} \cdot e\boldsymbol{E} = - \left.\frac{f_{\mathbf{k}}}{t}\right)_{\text{scattering}}$$

We now introduce a time constant τ called the relaxation time:

$$- \left.\frac{f_{\mathbf{k}}}{t}\right)_{\text{scattering}} = \frac{g_{\mathbf{k}}}{\tau}$$



This figure shows that at time $t = 0$, the distribution function is distorted by some external means. If the external force is removed, the electrons recover to the equilibrium distribution by collisions.

$$g_{\mathbf{k}} = - \left.\frac{f_{\mathbf{k}}}{t}\right)_{\text{scattering}} \cdot \tau$$

$$= \frac{-f^0}{E_{\mathbf{k}}} \tau \boldsymbol{v}_{\mathbf{k}} \cdot e\boldsymbol{E}$$

© Prof. Jasprit Singh www.eecs.umich.edu/~singh

BOLTZMANN TRANSPORT EQUATION: SHIFTED DISTRIBUTION

Using the relaxation time approximation

$$f_{\mathbf{k}} = f_{\mathbf{k}}^0 - \left(\frac{f_{\mathbf{k}}^0}{E_{\mathbf{k}}}\right) e\tau \boldsymbol{v}_{\mathbf{k}} \cdot \boldsymbol{E}$$

$$= f_{\mathbf{k}}^0 - (\nabla_{\mathbf{k}} f_{\mathbf{k}}^0) \cdot \frac{\boldsymbol{k}}{E_{\mathbf{k}}} \cdot e\tau \boldsymbol{v}_{\mathbf{k}} \cdot \boldsymbol{E}$$

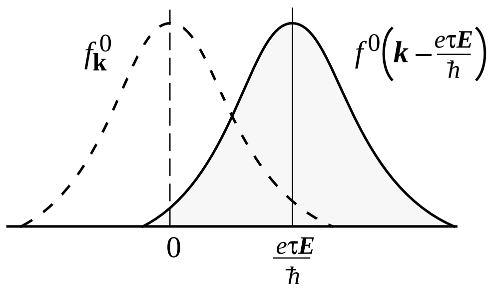
Using the relation

$$\hbar \frac{\mathbf{k}}{E_{\mathbf{k}}} \cdot \boldsymbol{v}_{\mathbf{k}} = 1$$

We have

$$f_{\mathbf{k}} = f_{\mathbf{k}}^0 - (\nabla_{\mathbf{k}} f_{\mathbf{k}}^0) \cdot \frac{e\tau \boldsymbol{E}}{\hbar}$$

$$= f_{\mathbf{k}}^0 \left(\boldsymbol{k} - \frac{e\tau \boldsymbol{E}}{\hbar}\right)$$



Change in carrier momentum:

$$\delta p = \hbar \delta \boldsymbol{k} = -e\tau \boldsymbol{E}$$

$$\delta v = -\frac{e\tau \boldsymbol{E}}{m^*}$$

This gives, for the mobility,

$$\mu = \frac{e\tau}{m^*}$$

If the electron concentration is n, the current density is

$$\boldsymbol{J} = ne\delta v$$

$$= \frac{ne^2 \tau \boldsymbol{E}}{m^*}$$

or the conductivity of the system is

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

This equation relates a microscopic quantity τ to a macroscopic quantity σ.

© Prof. Jasprit Singh www.eecs.umich.edu/~singh

How do we obtain the relaxation time τ?

Elastic collisions:

$$E(\boldsymbol{k}) = E(\boldsymbol{k}')$$

Alloy scatering, ionized impurity scattering, interface roughness scattering...are elastic processes.

According to the principle of microscopic reversibility:

$$W(\boldsymbol{k},\boldsymbol{k}') = W(\boldsymbol{k}',\boldsymbol{k})$$

The collision integral is now simplified as

$$\left.\frac{\partial f}{\partial t}\right)_{\text{scattering}} = \int \left[f(\boldsymbol{k}') - f(\boldsymbol{k})\right] W(\boldsymbol{k},\boldsymbol{k}') \frac{d^3\boldsymbol{k}'}{(2\pi)^3}$$

$$= \int \left[g(\boldsymbol{k}') - g(\boldsymbol{k})\right] W(\boldsymbol{k},\boldsymbol{k}') \frac{d^3\boldsymbol{k}'}{(2\pi)^3}$$

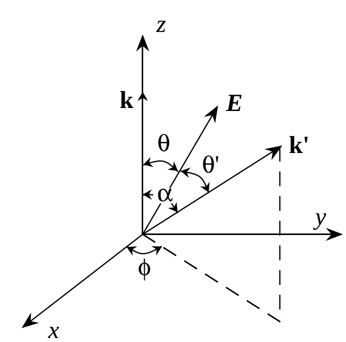
The simple form of the Boltzmann equation is

$$\frac{-\partial f^0}{\partial E_{\mathbf{k}}} \boldsymbol{v}_{\mathbf{k}} \cdot e\boldsymbol{E} = \int (g_{\mathbf{k}} - g_{\mathbf{k}'})\, W(\boldsymbol{k},\boldsymbol{k}') \frac{d^3\boldsymbol{k}'}{(2\pi)^3}$$

$$= \left.\frac{-\partial f}{\partial t}\right)_{\text{scattering}}$$

$$g_{\mathbf{k}} = \left(\frac{-\partial f^0}{\partial E}\right) e\boldsymbol{E} \cdot \boldsymbol{v}_{\mathbf{k}} \cdot \tau$$

$$= \left.\frac{-\partial f}{\partial t}\right)_{\text{scattering}} \cdot \tau$$



Coordinate system illustrating a scattering event.

Substituting this value in the integral on the right-hand side, we get

$$\frac{-\partial f^0}{\partial E_{\mathbf{k}}} \boldsymbol{v}_{\mathbf{k}} \cdot e\boldsymbol{E} = \frac{-\partial f^0}{\partial E_{\mathbf{k}}} e\tau\boldsymbol{E} \cdot \int (\boldsymbol{v}_{\mathbf{k}} - \boldsymbol{v}_{\mathbf{k}'})\, W(\boldsymbol{k},\boldsymbol{k}') \frac{d^3\boldsymbol{k}'}{(2\pi)^3}$$

or

$$\boldsymbol{v}_{\mathbf{k}} \cdot \boldsymbol{E} = \tau \int (\boldsymbol{v}_{\mathbf{k}} - \boldsymbol{v}_{\mathbf{k}'})\, W(\boldsymbol{k},\boldsymbol{k}')\, d^3\boldsymbol{k}' \cdot \boldsymbol{E}$$

and

$$\frac{1}{\tau} = \int W(\boldsymbol{k},\boldsymbol{k}') \left[1 - \frac{\boldsymbol{v}_{\mathbf{k}'} \cdot E}{\boldsymbol{v}_{\mathbf{k}} \cdot E}\right] \frac{d^3\boldsymbol{k}'}{(2\pi)^3} = \int W(\boldsymbol{k},\boldsymbol{k}') \left[1 - \frac{\cos\theta'}{\cos\theta}\right] \frac{d^3\boldsymbol{k}'}{(2\pi)^3}$$

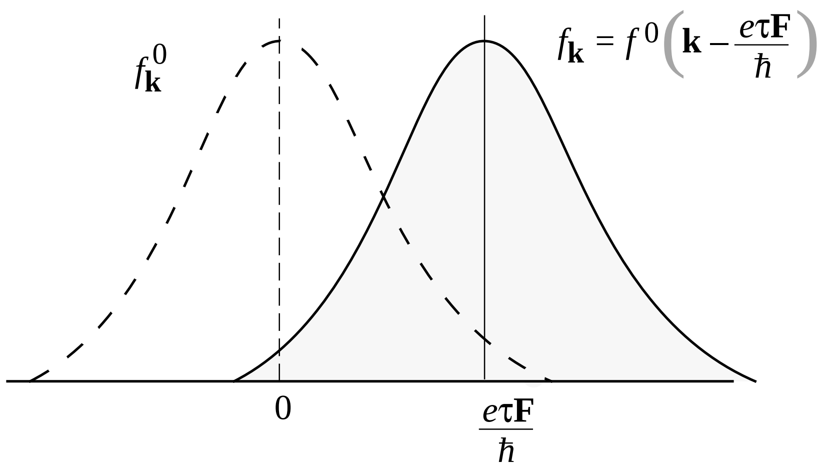
$$= \int W(\boldsymbol{k},\boldsymbol{k}')(1 - \cos\alpha) \frac{d^3\boldsymbol{k}'}{(2\pi)^3}$$

$\Rightarrow$ The larger the scattering angle, α, the greater the effect on mobility.

© Prof. Jasprit Singh www.eecs.umich.edu/~singh

MICROSCOPIC VERSUS MACROSCOPIC: AVERAGING PROCEDURES FOR DRIFT MOBILITY

An experiment measures the averaged response of all electrons—how does one go from scattering time of a single electron to the average value for an ensemble?



The displaced distribution function shows the effect of an applied electric field.

Drift current:

$$J = \int e\, v_k f_k \frac{d^3k}{(2\pi)^3}$$

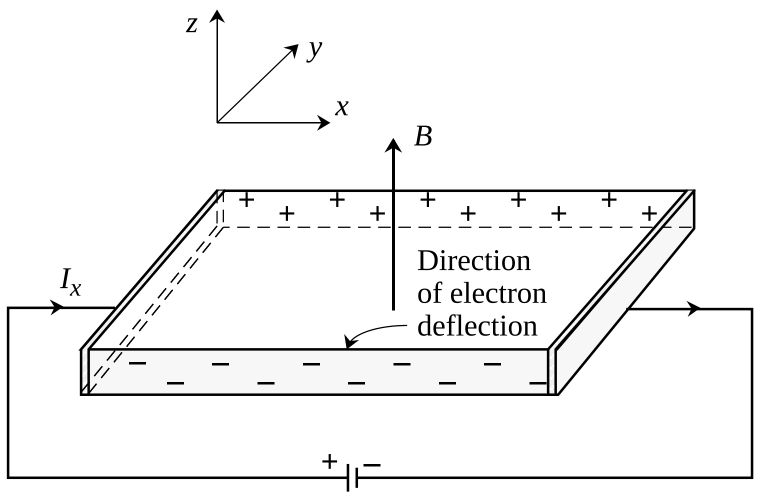
$$\langle J_x \rangle = \frac{ne^2}{m^*} \frac{\langle E\tau \rangle}{\langle E \rangle} \quad ; \mu = \frac{e}{m^*} \frac{\langle E\tau \rangle}{\langle E \rangle}$$

< > averaging with respect to <u>equilibrium</u> distribution function

© Prof. Jasprit Singh www.eecs.umich.edu/~singh

TRANSPORT IN WEAK MAGENTIC FIELD: HALL MOBILITY

Why Hall Effect: Carrier density and Hall mobility can both be obtained



A rectangular Hall sample of an *n*-type semiconductor.

At low magnetic field:

$$\sigma_{xx} = \sigma_0 = \text{conductivity in the absence of a } B\text{-field}$$

$$\sigma_{xy} = \sigma_0 \mu_H B$$

Hall mobility: $\mu_H = \dfrac{\langle\langle \tau^2 \rangle\rangle}{\langle\langle \tau \rangle\rangle^2} \mu$; $\langle\langle A \rangle\rangle = \langle EA \rangle$

Hall factor: $r_H = \dfrac{\mu_H}{\mu}$

© Prof. Jasprit Singh www.eecs.umich.edu/~singh