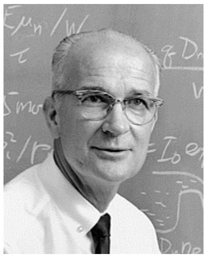
Handout 23

Electron Transport Equations

In this lecture you will learn:

- Position dependent non-equilibrium distribution functions
- The Liouville equation
- The Boltzmann equation
- Relaxation time approximation
- Transport equations



William Schockley
(1910-1989)

Note on Notation

In this handout, unless states otherwise, we will assume a conduction band with a dispersion given by:

$$E(\vec{k}) = E_c + \frac{\hbar^2}{2}\vec{k}^T . M^{-1} . \vec{k}$$

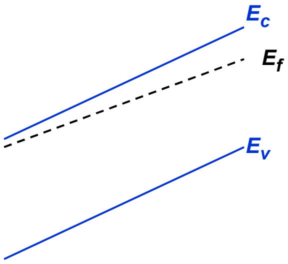
$$\Rightarrow \quad \vec{v}(\vec{k}) = M^{-1} . \hbar\, \vec{k}$$

In the presence of an electric field:

$$E(\vec{k},\vec{r}) = E_c(\vec{r}) + \frac{\hbar^2}{2}\vec{k}^T . M^{-1} . \vec{k}$$

where:

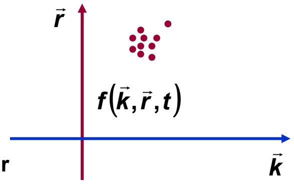
$$\nabla E_c(\vec{r}) = e\vec{E}$$



Position Dependent Non-Equilibrium Distribution Function

We generalize the concept of non-equilibrium distribution functions to situations where electron distributions could also be a function of position (as is the case in almost all electronic/optoelectronic devices):

$$f\left(\vec{k},\vec{r},t\right)$$



The local electron density is obtained upon integration over k-space:

$$n(\vec{r},t)=2\times\int_{\text{FBZ}}\frac{d^d\vec{k}}{(2\pi)^d}\,f\left(\vec{k},\vec{r},t\right)$$

Local Equilibrium Distribution Function:

Electrons at a given location are likely to reach thermal equilibrium among themselves much faster than with electrons in other locations. The local equilibrium distribution function is defined by a local Fermi-level in the following way:

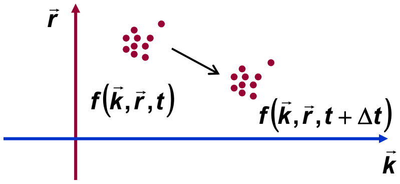
$$f_o\left(\vec{k},\vec{r},t\right)=\frac{1}{1+e^{\left(E\left(\vec{k},\vec{r}\right)-E_f(\vec{r},t)\right)/KT}}$$

with the condition that the local Fermi level must be chosen such that:

$$n(\vec{r},t)=2\times\int_{\text{FBZ}}\frac{d^d\vec{k}}{(2\pi)^d}\,f_o\left(\vec{k},\vec{r},t\right)=2\times\int_{\text{FBZ}}\frac{d^d\vec{k}}{(2\pi)^d}\,f\left(\vec{k},\vec{r},t\right)$$

Case of No Scattering: Liouville Equation

Question: How does the non-equilibrium distribution function behave in time in the absence of scattering?



Consider an initial non-equilibrium distribution 2*d* dimensions at time "*t*", as shown

There is also an applied electric field, as shown

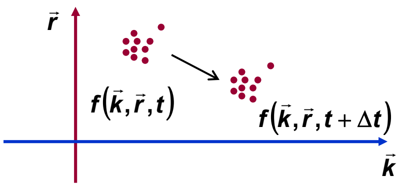
In time interval "Δt" each electron would have moved in k-space according to the dynamical equation:

$$\frac{d\,\hbar\vec{k}(t)}{dt}=-e\,\vec{E}\qquad\begin{cases}\vec{k}(t)=\text{initial momentum value}\\ \vec{k}(t+\Delta t)=\text{final momentum value}\end{cases}$$

But in the same time interval "Δt" each electron would have moved in real-space according to the equation:

$$\frac{d\,\vec{r}(t)}{dt}=\vec{v}\left(\vec{k}(t)\right)\qquad\begin{cases}\vec{r}(t)=\text{initial position value}\\ \vec{r}(t+\Delta t)=\text{final position value}\end{cases}$$

Case of No Scattering: Liouville Equation



$$\frac{d\,\hbar\vec{k}(t)}{dt} = -e\,\vec{E}$$

$$\frac{d\,\vec{r}(t)}{dt} = \vec{v}\big(\vec{k}(t)\big)$$

The distribution at time "$t+\Delta t$" must obey the equation:

$$f\big(\vec{k}(t+\Delta t),\vec{r}(t+\Delta t),t+\Delta t\big) = f\big(\vec{k}(t),\vec{r}(t),t\big)$$

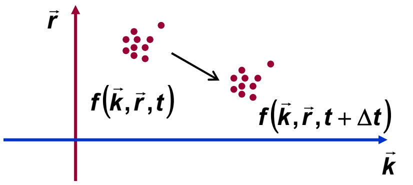
This is because in time "Δt" the electron with initial momentum $\vec{k}(t)$ and position $\vec{r}(t)$ would have gone over to the state with momentum $\vec{k}(t+\Delta t)$ and position $\vec{r}(t+\Delta t)$

$$f\big(\vec{k}(t+\Delta t),\vec{r}(t+\Delta t),t+\Delta t\big) = f\big(\vec{k}(t),\vec{r}(t),t\big)$$

$$\Rightarrow \quad f\left(\vec{k}+\frac{d\vec{k}(t)}{dt}\Delta t,\vec{r}+\frac{d\vec{r}(t)}{dt}\Delta t,t+\Delta t\right) = f\big(\vec{k},\vec{r},t+\Delta t\big)$$

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

Case of No Scattering: Liouville Equation



$$\frac{d\,\hbar\vec{k}(t)}{dt} = -e\,\vec{E}$$

$$\frac{d\,\vec{r}(t)}{dt} = \vec{v}\big(\vec{k}(t)\big)$$

We have:

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

The above equation implies that the underlined term must be zero:

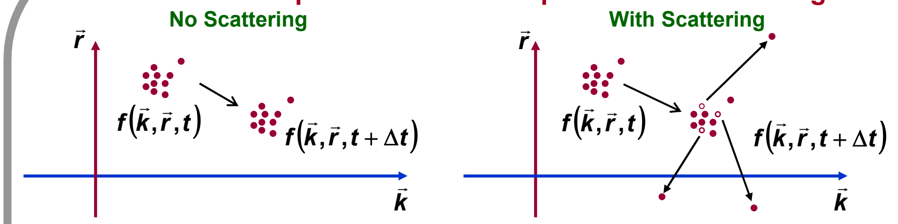
$$\boxed{\frac{\partial f(\vec{k},\vec{r},t)}{\partial t}+\nabla_{\vec{k}}f(\vec{k},\vec{r},t).\,\frac{d\vec{k}(t)}{dt}+\nabla_{\vec{r}}f(\vec{k},\vec{r},t).\,\frac{d\vec{r}(t)}{dt}=0} \longrightarrow$$

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

Liouville equation

Describes the deterministic evolution of electron distribution in k-space and real-space

Boltzmann Equation: Liouville Equation with Scattering



Now we have:

$$f(\vec k(t+\Delta t),\vec r(t+\Delta t),t+\Delta t) = f(\vec k(t),\vec r(t),t) + \{\text{ changes due to scattering }\}\Delta t$$

$$\Rightarrow \boxed{\underbrace{\frac{\partial f(\vec k,\vec r,t)}{\partial t} + \nabla_{\vec k} f(\vec k,\vec r,t)\,.\,\frac{d\vec k(t)}{dt} + \nabla_{\vec r} f(\vec k,\vec r,t)\,.\,\vec v(\vec k)}_{\text{Deterministic evolution}} = \underbrace{\{\text{ changes due to scattering}\}}_{\text{Non-deterministic evolution}}}$$

Boltzmann's equation

Boltzmann Equation: Relaxation Time Approximation

$$\frac{\partial f(\vec k,\vec r,t)}{\partial t} + \nabla_{\vec k} f(\vec k,\vec r,t)\,.\,\frac{d\vec k(t)}{dt} + \nabla_{\vec r} f(\vec k,\vec r,t)\,.\,\vec v(\vec k) = \{\text{ changes due to scattering}\}$$

Local Equilibrium:

- Scattering is local in space – i.e. electrons at one location do not scatter from impurities, defects, phonons, and other electrons that are present at another location

- Scattering restores local equilibrium – i.e. it drives the distribution function at any location to the local equilibrium distribution function at that location

$$\{\text{ changes due to scattering}\} = -\frac{\left[f(\vec k,\vec r,t) - f_o(\vec k,\vec r,t)\right]}{\tau}$$

Note that: $n(\vec r,t) = 2\times\int_{\text{FBZ}} \frac{d^d\vec k}{(2\pi)^d} f(\vec k,\vec r,t) = 2\times\int_{\text{FBZ}} \frac{d^d\vec k}{(2\pi)^d} f_o(\vec k,\vec r,t)$

$$\Rightarrow \boxed{\frac{\partial f(\vec k,\vec r,t)}{\partial t} + \nabla_{\vec k} f(\vec k,\vec r,t)\,.\,\frac{d\vec k(t)}{dt} + \nabla_{\vec r} f(\vec k,\vec r,t)\,.\,\vec v(\vec k) = -\frac{\left[f(\vec k,\vec r,t) - f_o(\vec k,\vec r,t)\right]}{\tau}}$$

Boltzmann equation in the relaxation time approximation

Transport Equations: Continuity Equation

Boltzmann equation can be manipulated to give simpler transport equations

$$\frac{\partial f(\vec{k},\vec{r},t)}{\partial t}+\nabla_{\vec{k}} f(\vec{k},\vec{r},t)\,.\,\frac{d\vec{k}(t)}{dt}+\nabla_{\vec{r}} f(\vec{k},\vec{r},t)\,.\,\vec{v}(\vec{k})=-\frac{\left[f(\vec{k},\vec{r},t)-f_o(\vec{k},\vec{r},t)\right]}{\tau}$$

Integrate LHS and RHS over k-space, multiply by two, and use:

$$n(\vec{r},t)=2\times\int_{\text{FBZ}}\frac{d^d\vec{k}}{(2\pi)^d}\,f(\vec{k},\vec{r},t)=2\times\int_{\text{FBZ}}\frac{d^d\vec{k}}{(2\pi)^d}\,f_o(\vec{k},\vec{r},t)$$

$$\vec{J}(\vec{r},t)=2\,(-e)\times\int_{\text{FBZ}}\frac{d^d\vec{k}}{(2\pi)^d}\,f(\vec{k},\vec{r},t)\,\vec{v}(\vec{k})$$

$$2\times\int_{\text{FBZ}}\frac{d^d\vec{k}}{(2\pi)^d}\,\nabla_{\vec{k}} f(\vec{k},\vec{r},t)\,.\,\frac{d\vec{k}(t)}{dt}=0$$

$$\left\{\frac{d\,\hbar\vec{k}(t)}{dt}=-e\,\vec{E}\right.$$

to get:

$$\boxed{\frac{\partial n(\vec{r},t)}{\partial t}-\frac{1}{e}\nabla\,.\,\vec{J}(\vec{r},t)=0}\longrightarrow$$

Continuity equation

Transport Equations: Current Density Equation

Assume DC applied electric field and steady state:

$$\left\{\frac{d\,\hbar\vec{k}(t)}{dt}=-e\,\vec{E}\right.$$

$$\cancelto{0}{\frac{\partial f(\vec{k},\vec{r},t)}{\partial t}}+\nabla_{\vec{k}} f(\vec{k},\vec{r},t)\,.\,\frac{d\vec{k}(t)}{dt}+\nabla_{\vec{r}} f(\vec{k},\vec{r},t)\,.\,\vec{v}(\vec{k})=-\frac{\left[f(\vec{k},\vec{r},t)-f_o(\vec{k},\vec{r},t)\right]}{\tau}$$

$$\Rightarrow -e\,\nabla_{\vec{k}} f(\vec{k},\vec{r})\,.\,\frac{\vec{E}}{\hbar}+\nabla_{\vec{r}} f(\vec{k},\vec{r})\,.\,\vec{v}(\vec{k})=-\frac{\left[f(\vec{k},\vec{r})-f_o(\vec{k},\vec{r})\right]}{\tau}$$

$$\Rightarrow e\tau\,\nabla_{\vec{k}} f(\vec{k},\vec{r})\,.\,\frac{\vec{E}}{\hbar}-\tau\,\nabla_{\vec{r}} f(\vec{k},\vec{r})\,.\,\vec{v}(\vec{k})=f(\vec{k},\vec{r})-f_o(\vec{k},\vec{r})$$

$$\Rightarrow f(\vec{k},\vec{r})=f_o(\vec{k},\vec{r})+e\frac{\tau}{\hbar}\,\nabla_{\vec{k}} f(\vec{k},\vec{r})\,.\,\vec{E}-\tau\,\nabla_{\vec{r}} f(\vec{k},\vec{r})\,.\,\vec{v}(\vec{k})$$

Assumption:

Since the difference between $f(\vec{k},\vec{r})$ and $f_o(\vec{k},\vec{r})$ will be of the order of the applied field, it is safe replace $f(\vec{k},\vec{r})$ by $f_o(\vec{k},\vec{r})$ on the RHS in the above equation:

$$\Rightarrow f(\vec{k},\vec{r})\approx f_o(\vec{k},\vec{r})+e\frac{\tau}{\hbar}\,\nabla_{\vec{k}} f_o(\vec{k},\vec{r})\,.\,\vec{E}-\tau\,\nabla_{\vec{r}} f_o(\vec{k},\vec{r})\,.\,\vec{v}(\vec{k})$$

Transport Equations: Current Density Equation

$$\Rightarrow f(\vec{k},\vec{r}) \approx f_o(\vec{k},\vec{r}) + e\frac{\tau}{\hbar}\nabla_{\vec{k}} f_o(\vec{k},\vec{r}) . \vec{E} - \tau \nabla_{\vec{r}} f_o(\vec{k},\vec{r}) . \vec{v}(\vec{k})$$

Multiply both sides by $2\,(-e)\,\vec{v}(\vec{k})$ and integrate over k-space to get:

LHS:

$$2\,(-e) \times \int_{FBZ} \frac{d^d\vec{k}}{(2\pi)^d} f(\vec{k},\vec{r})\,\vec{v}(\vec{k})$$

$$= \vec{J}(\vec{r})$$

RHS:

First note that: $f_o(\vec{k},\vec{r}) = \dfrac{1}{1+e^{(E(\vec{k},\vec{r})-E_f(\vec{r}))/KT}}$

$$\Rightarrow \nabla_{\vec{r}}\, f_o(\vec{k},\vec{r}) . \vec{v}(\vec{k}) = \frac{\partial f_o(\vec{k},\vec{r})}{\partial E} \nabla_{\vec{r}}\, [E_c(\vec{r}) - E_f(\vec{r})] . \frac{1}{\hbar}\nabla_{\vec{k}} E(\vec{k})$$

$$= \frac{1}{\hbar}\nabla_{\vec{k}} f_o(\vec{k},\vec{r}) . \nabla_{\vec{r}}\, [E_c(\vec{r}) - E_f(\vec{r})]$$

Therefore the RHS can be written compactly as:

$$2(-e) \times \int_{FBZ} \frac{d^d\vec{k}}{(2\pi)^d} \left\{ f_o(\vec{k},\vec{r}) + \nabla_{\vec{k}} f(\vec{k},\vec{r}) . \left[\frac{e\tau}{\hbar}\vec{E} - \frac{\tau}{\hbar}\nabla_{\vec{r}}\, [E_c(\vec{r}) - E_f(\vec{r})] \right] \right\} \vec{v}(\vec{k})$$

$$\approx 2(-e) \times \int_{FBZ} \frac{d^d\vec{k}}{(2\pi)^d} f_o\left(\vec{k} + \frac{e\tau}{\hbar}\vec{E} - \frac{\tau}{\hbar}\nabla_{\vec{r}}\, [E_c(\vec{r}) - E_f(\vec{r})], \vec{r} \right) \vec{v}(\vec{k})$$

Transport Equations: Current Density Equation

$$\approx 2(-e) \times \int_{FBZ} \frac{d^d\vec{k}}{(2\pi)^d} f_o\left(\vec{k} + \frac{e\tau}{\hbar}\vec{E} - \frac{\tau}{\hbar}\nabla_{\vec{r}}[E_c(\vec{r}) - E_f(\vec{r})], \vec{r} \right) \vec{v}(\vec{k})$$

$$= 2(-e) \times \int_{FBZ} \frac{d^d\vec{k}}{(2\pi)^d} f_o(\vec{k},\vec{r})\,\vec{v}\left(\vec{k} - \frac{e\tau}{\hbar}\vec{E} + \frac{\tau}{\hbar}\nabla_{\vec{r}}[E_c(\vec{r}) - E_f(\vec{r})] \right)$$

For the conduction band of a semiconductor with parabolic dispersion:

$$\vec{v}(\vec{k}) = M^{-1} . \hbar\,\vec{k}$$

The RHS becomes:

$$2(-e) \times \int_{FBZ} \frac{d^d\vec{k}}{(2\pi)^d} f_o(\vec{k},\vec{r})\,M^{-1} . \hbar\left(\cancelto{0}{\vec{k}} - \frac{e\tau}{\hbar}\vec{E} + \frac{\tau}{\hbar}\nabla_{\vec{r}}[E_c(\vec{r}) - E_f(\vec{r})] \right)$$

$$= n(\vec{r})e^2\tau\, M^{-1} . \left[\vec{E} - \frac{1}{e}\nabla_r[E_c(\vec{r}) - E_f(\vec{r})] \right] = \overline{\overline{\sigma}} . \vec{E} - \frac{1}{e}\overline{\overline{\sigma}} . \nabla_{\vec{r}}[E_c(\vec{r}) - E_f(\vec{r})]$$

Finally putting together the **LHS** and the **RHS** we get:

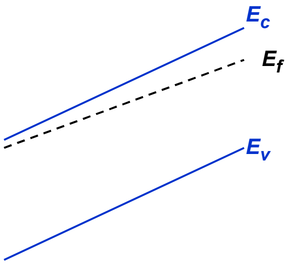
$$\boxed{\vec{J}(\vec{r}) = \overline{\overline{\sigma}} . \left(\vec{E} - \frac{1}{e}\nabla_{\vec{r}}[E_c(\vec{r}) - E_f(\vec{r})] \right)} \longrightarrow \text{Current density equation}$$

Current Density and the Fermi Level (Chemical Potential)

The expression for the current density is:

$$\vec{J}(\vec{r}) = \overline{\overline{\sigma}} \,.\left(\vec{E} - \frac{1}{e}\nabla_{\vec{r}}\left[E_c(\vec{r}) - E_f(\vec{r})\right]\right)$$

Therefore, currents can flow as a result of both potential gradients and Fermi-level (or chemical potential) gradients



Since:

$$\nabla E_c(\vec{r}) = e\vec{E}$$

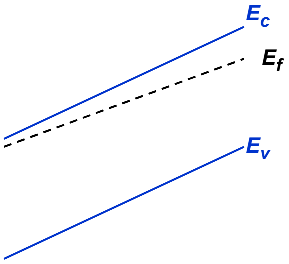
We get:

$$\vec{J}(\vec{r}) = \overline{\overline{\sigma}} \,.\frac{1}{e}\nabla_{\vec{r}} E_f(\vec{r})$$

Therefore, currents flow ONLY as a result of gradients in the Fermi level (or the chemical potential)

Transport Equations: Drift and Diffusion

The current density equation:



$$\vec{J}(\vec{r}) = \overline{\overline{\sigma}} \,.\left(\vec{E} - \frac{1}{e}\nabla_{\vec{r}}\left[E_c(\vec{r}) - E_f(\vec{r})\right]\right)$$

can be cast in one more form that is more common

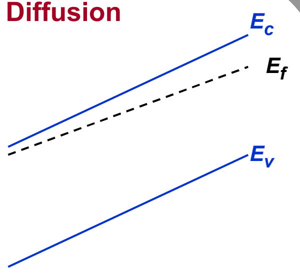
We start by relating the gradient in the Fermi level to the gradient in the carrier density:

$$n(\vec{r}) = 2\times \int_{\text{FBZ}} \frac{d^d\vec{k}}{(2\pi)^d}\, f_o(\vec{k},\vec{r})$$

$$\Rightarrow \nabla_{\vec{r}}\, n(\vec{r}) = 2\times \int_{\text{FBZ}} \frac{d^d\vec{k}}{(2\pi)^d}\, \nabla_{\vec{r}} f_o(\vec{k},\vec{r}) = 2\times \int_{\text{FBZ}} \frac{d^d\vec{k}}{(2\pi)^d}\, \frac{\partial f_o(\vec{k},\vec{r})}{\partial E}\nabla_{\vec{r}}\left[E_c(\vec{r}) - E_f(\vec{r})\right]$$

$$= -\left(2\times \int_{\text{FBZ}} \frac{d^d\vec{k}}{(2\pi)^d}\; - \frac{\partial f_o(\vec{k},\vec{r})}{\partial E}\right)\nabla_{\vec{r}}\left[E_c(\vec{r}) - E_f(\vec{r})\right]$$

Transport Equations: Drift and Diffusion



The expression for the current density becomes:

$$\vec{J}(\vec{r}) = \overline{\overline{\sigma}} \cdot \vec{E} - \frac{1}{e}\overline{\overline{\sigma}} \cdot \nabla_{\vec{r}}[E_c(\vec{r}) - E_f(\vec{r})]$$

$$= \overline{\overline{\sigma}} \cdot \vec{E} + \frac{1}{e}\frac{\overline{\overline{\sigma}}}{2\int_{FBZ}\frac{d^d\vec{k}}{(2\pi)^d}\left(-\frac{\partial f_o(\vec{k},\vec{r})}{\partial E}\right)} \cdot \nabla_{\vec{r}} n(\vec{r})$$

$$\boxed{\vec{J}(\vec{r}) = \overline{\overline{\sigma}} \cdot \vec{E} + e\,\overline{\overline{D}} \cdot \nabla_{\vec{r}} n(\vec{r})} \longrightarrow$$

Current density equation

Where we have the defined the diffusivity tensor as:

$$\overline{\overline{D}} = \frac{1}{e^2}\frac{\overline{\overline{\sigma}}}{2\int_{FBZ}\frac{d^d\vec{k}}{(2\pi)^d}\left(-\frac{\partial f_o(\vec{k},\vec{r})}{\partial E}\right)}$$

$$\left\{ \overline{\overline{\sigma}} = n(\vec{r}) e^2 \tau M^{-1} \right.$$

The current density equation shows that current can result from drift when there is an electric field (the first term on the RHS) and also by diffusion if there is a carrier density gradient (the second term on the RHS)

Diffusivity, Conductivity, and Mobility - I

We define the mobility tensor as:

$$\overline{\overline{\mu}} = e\tau M^{-1}$$

$$\left\{ \overline{\overline{\sigma}}(\vec{r}) = n(\vec{r})\, e\, \overline{\overline{\mu}} \right.$$

Einstein Relation:

Conductivity and diffusivity are related by the Einstein relation:

$$\overline{\overline{D}} = \frac{1}{e^2}\frac{\overline{\overline{\sigma}}}{2\int_{FBZ}\frac{d^d\vec{k}}{(2\pi)^d}\left(-\frac{\partial f_o(\vec{k},\vec{r})}{\partial E}\right)}$$

Example - Semiconductors:

Consider a semiconductor at high temperatures and assume that Maxwell-Boltzmann statistics apply:

$$f_o(\vec{k},\vec{r}) = \frac{1}{1+e^{(E(\vec{k})-E_f(\vec{r}))/KT}} \approx e^{-(E(\vec{k})-E_f(\vec{r}))/KT}$$

$$\left\{ E_c - E_f >> KT \right.$$

Then:

$$2\int_{FBZ}\frac{d^d\vec{k}}{(2\pi)^d}\left(-\frac{\partial f_o(\vec{k},\vec{r})}{\partial E}\right) = \frac{n(\vec{r})}{KT}$$

and the Einstein relation can be expressed as:

$$\overline{\overline{D}} = \frac{1}{e^2}\frac{\overline{\overline{\sigma}}}{n(\vec{r})/KT} = \frac{KT}{e}\left[e\tau M^{-1}\right] = \frac{KT}{e}\overline{\overline{\mu}}$$

Diffusivity, Conductivity, and Mobility - II

Example - Metals:

Consider a metal or a highly doped semiconductor at low temperatures. Then:

$$-\frac{\partial f_o(\vec{k},\vec{r})}{\partial E} \approx \delta\left(E(\vec{k})-E_f\right)$$

And:

$$2\int_{FBZ} \frac{d^d\vec{k}}{(2\pi)^d}\left(-\frac{\partial f_o(\vec{k},\vec{r})}{\partial E}\right) = g_{dD}(E_f)$$

and the Einstein relation becomes:

$$\overline{\overline{D}} = \frac{1}{e^2}\frac{\overline{\overline{\sigma}}}{g_{dD}(E_f)}$$