University of California, Berkeley
EE230 - Solid State Electronics *Prof. J. Bokor*

Transport Theory

(read Lundstrom 3.1 - 3.4)

Aim Develop a general approach for relating microscopic description of carrier motion to macroscopic description.

Drift-Diffusion equation:

Classical approach to device design

$$\underbrace{\text{material properties: } \mu,\ D}_{\underline{\text{microphysics is buried in here}}} \quad + \quad \underbrace{\text{Boundary conditions}}_{\text{device structure}}$$

Device behavior described by independent specification of material and structure.

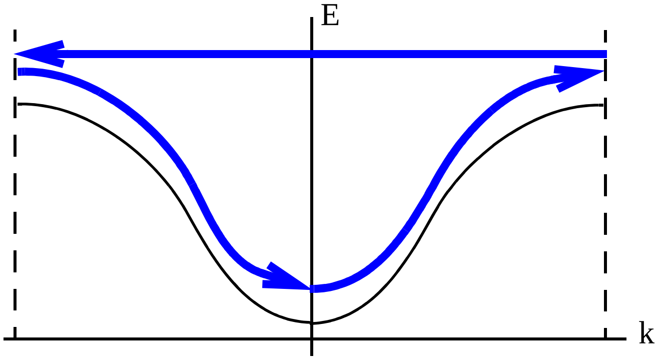
Modern devices

μ, D: can't bury microphysics (i.e. ballistic transport)
also depend explicitly on device structure (i.e. nonlocal transport)

Carrier energy & momentum distributions vary strongly in devices

Carrier scattering: key to transport.

Paradox: no scattering --> net J=0!



consider simple band $E = E_o - E_o \cos(ka)$

$$v = \frac{1}{\hbar}\frac{\partial E}{\partial K} = \frac{E_o a}{\hbar}\sin(ka)$$

periodic motion - Bloch oscillation. This has been experimentally observed in superlattices [“Coherent submillimeter-wave emission from Bloch oscillations in a semiconductor superlattice,” C. Waschke, et al., Phys. Rev. Lett. 70, 3319 - 3322 (1993). PDF copy is posted on the class web site.]

Electrons oscillate through BZ [Bragg diffraction] → localized in real space → no net current!

Scattering damps oscillation resulting in a net motion in an applied field. Yet the motion is damped by scattering. The message is that **transport depends on the balance between the applied driving force and dissipation by scattering forces**.

Boltzmann transport equation

Semi-classical approach. In semiconductors, all the QM is buried in m*. Electron motion will be described by classical mechanics, except that scattering probabilities will also be derived using quantum mechanics.

Complete description: could solve Newton equations for each particle (electron):

$$\frac{dp_i}{dt} = qE + \mathcal{F}(r, p, t)$$

random forces due to
phonons, impurities

for all $i = 1, \ldots, N$. This is clearly not feasible.

Instead, we take a statistical approach:
define distribution function (single particle):

$f(\vec{r}, \vec{p}, t)$: probability of finding a particle at $\vec{r}$, with momentum $\vec{p}$ at time t.

“phase space”: 6 dimensional space - x, y, z, p_x, p_y, p_z

The particle density is found as:

Since momentum is discrete, we show a summation over allowed values of p. However, it is more convenient to convert to an appropriate integral.

$$\frac{1}{V}\sum_{p} f(\vec{r},\vec{p}) \rightarrow \frac{1/V}{\left[\begin{array}{l}\text{vol of}\\ \text{one state in}\\ \text{p-space}\end{array}\right]}\iiint_{\text{1st BZ}} f(r,p)\,d^3p$$

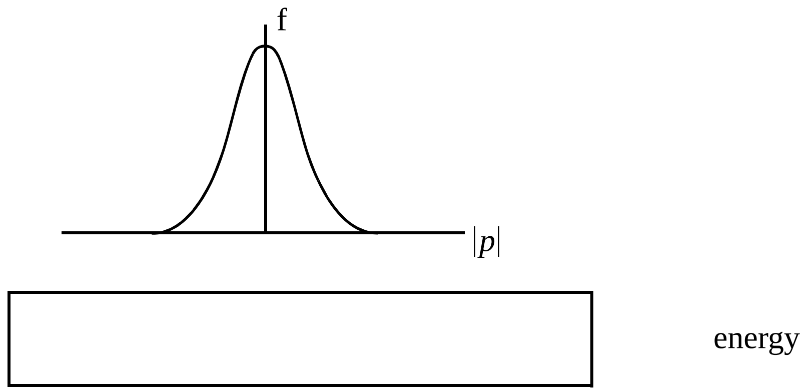
$$\left[\begin{array}{l}\text{vol of}\\ \text{one state in}\\ \text{p-space}\end{array}\right] \leftarrow \frac{1}{2}\left(\frac{2\pi}{L}\hbar\right)^3$$

$$\cong \frac{1}{4\pi^3\hbar^3}\int\int\int_{-\infty}^{\infty} f(r,p)\,d^3p$$

(since *f* is well localized inside the 1st BZ)

[This general method of converting from a sum in p-space to an integral is important, and will come up again and again.]

Example: MB distribution:



$$f(r,p) \;=\; \exp\{[E_F - E_c(r)]/kT\}\exp[-p^2/(2m^*kT)]$$

to get the carrier density, integrate over momentum space

$$n(r) \;=\; \frac{1}{4\pi^3\hbar^3}\int_{\text{1st BZ}} \exp[E_F - E_c(r) - p^2/2m^*/kT]\,d^3p$$

$$= \frac{1}{4\pi^3\hbar^3}\exp[(E_F - E_c)/kT]\int e^{-p^2/2m^*kT}d^3p$$

for reasonable T, only populated near bottom of band, so we can extend the integral over all p-space

$$\underset{\text{p-space}}{\iiint} e^{-p^2/2m^*kT} p^2 \, dp \, d\Omega$$

Thus, the integral is:

Now use:

$$\int_0^\infty x^2 e^{-\alpha x^2} dx = \frac{1}{4\alpha}\sqrt{\frac{\pi}{\alpha}}$$

Finally:

$$n = \frac{1}{4}\left[\frac{2m^*kT}{\pi\hbar^2}\right]^{3/2} \exp[(E_F - E_c)/kT]$$

$$\boxed{= N_c \exp[(E_F - E_c)/kT]}$$

which is our previous result.

Average kinetic energy density:

$$W(r) = \frac{1}{4\pi^3\hbar^3}\int \frac{p^2}{2m^*} \exp\{[E_F - E_c - p^2/2m^*]/kT\} d^3p$$

$$= \frac{1}{8\pi^3\hbar^3} 4\pi \exp[(E_F - E_c)/kT] \underbrace{\int_0^\infty dp\, p^4 e^{-p^2/2m^*kT}}_{\frac{3}{8}\pi^{1/2}(2m^*kT)^{5/2}}$$

$$= \left(\frac{3}{2}kT\right)\frac{1}{4}\left(\frac{2m^*kT}{\pi\hbar^2}\right)^{3/2} \exp[(E_F - E_c)/kT]$$

So we can say that the energy / electron = $\frac{W}{n} = \frac{3}{2}kT$. Again, a familiar result.

How about current density?

$$\vec{J}(r) = \frac{q}{4\pi^3\hbar^3}\int_p \frac{\vec{p}}{m^*}\exp\left\{\left[E_F - E_c - \frac{p^2}{2m^*}\right]/kT\right\}d^3p$$

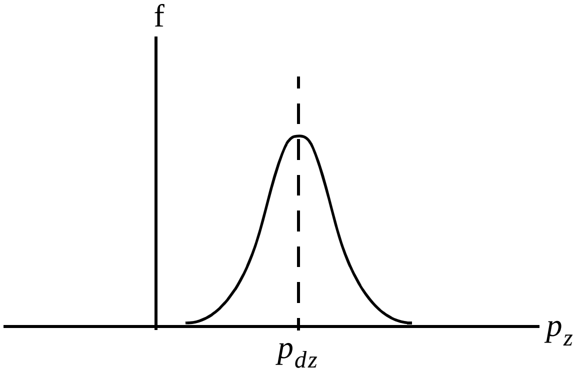
$$= 0$$

thermal equilibrium, *f* is even → $J = 0$

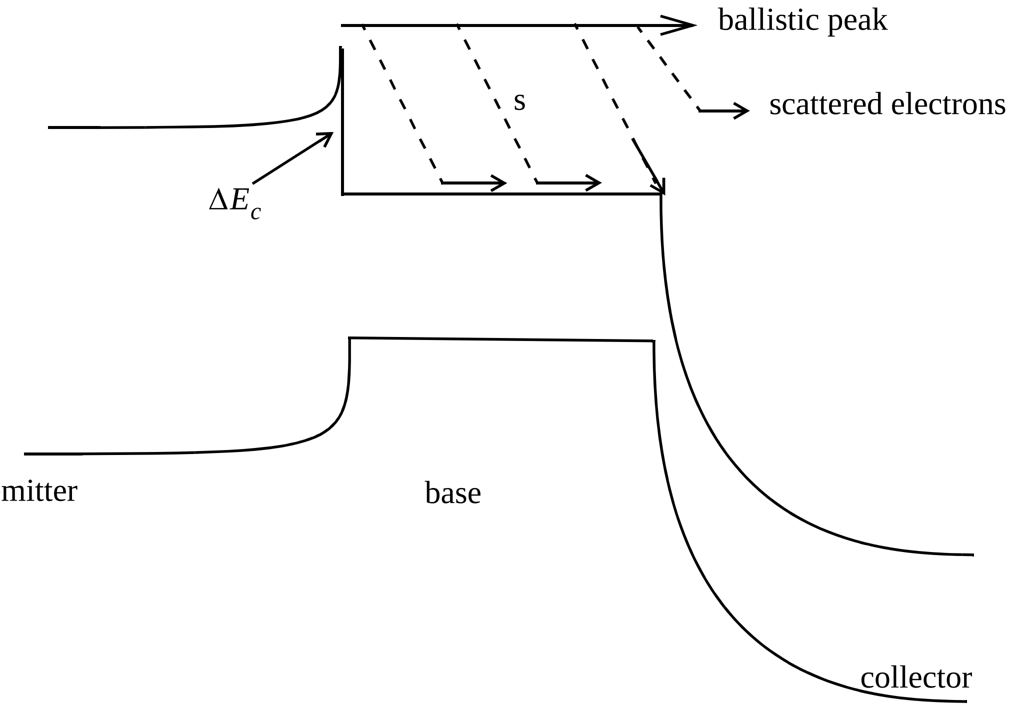
Very common and useful guess for *f* in nonequilibrium conditions is the “drifted” Maxwellian:

$$f(r, p, t) = \exp\left[\left(\underset{\substack{\uparrow \\ \text{quasi-Fermi level}}}{F_n(r, t)} - E_c - \frac{|\vec{p} - \vec{p}_d|^2}{2m^*}\right)/kT\right]$$

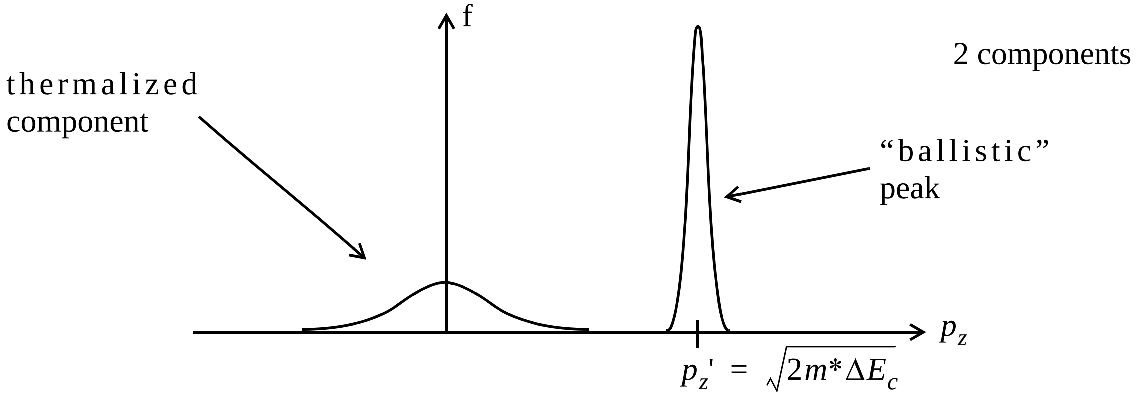
“drift” velocity



Consider heterojunction bipolar transistor (HBT) band diagram



electron distribution function at collector



How could we calculate such a distribution?

"Conservation of probability" --> continuity eqn for *f*.

<u>Balance</u> forces and scattering

$$\frac{df(r,p,t)}{dt} = \left.\frac{\partial f}{\partial t}\right|_{G-R}$$

total derivative:
all changes in *f*

driving terms:
generation, recombination, scattering

To see how this is used, expand total derivative using the chain rule:

$$\frac{df}{dt} = \frac{d\vec{r}}{dt}\vec{\nabla}_r f + \frac{d\vec{p}}{dt}\vec{\nabla}_p f + \frac{\partial f}{\partial t}$$

Use $\vec{F} = \frac{d\vec{p}}{dt}$.

This is known as the Boltzmann transport equation (BTE). Compare this to the carrier continuity eqn:

$$\frac{\partial n}{\partial t} + \frac{1}{q}\vec{\nabla}\cdot J = \left.\frac{\partial n}{\partial t}\right|_{G-R}$$

We can rewrite the BTE to highlight the analogy to carrier continuity:

$$\frac{\partial f}{\partial t} + \vec{\nabla}_r\cdot(\vec{v}f) + \vec{\nabla}_p\cdot(\vec{F}f) = \left.\frac{\partial f}{\partial t}\right|_{G-R}$$

This shows how the BTE is a continuity equation for *f*. The $\vec{v}f$ term is analogous to an intuitively appealing probability <u>current</u> in real space. The less intuitive element here is the $\vec{F}f$ term, which represents the probability current in momentum space.

Now let's examine the term: $\left.\frac{\partial f}{\partial t}\right|_{G-R}$

2 processes contribute.

1. <u>Actual generation-recombination processes</u> such as photogeneration, defect recombination, stimulated emission, ...

   explicitly write s(r, p, t) for these

2. <u>Carrier scattering.</u> This takes carriers from one momentum state to another - creates sources-sinks in momentum space.

Write $\left.\frac{\partial f}{\partial t}\right|_{coll}$ for these processes.

For transport problems, we will be mainly interested in collisions.

Collision integral

Consider the effect of collisions on the distribution at a particular point in phase space: *f(p, r, t).* Two types of collision processes affect *f* at this point:

(1) carriers at p' scatter into p
(2) carriers at p scatter out to p'

The collision rate for process (1) is given by:

$$\underset{\substack{\nearrow\\ \text{prob. of finding}\\ \text{a carrier at } p'}}{f(p')}\underset{\substack{\uparrow\\ \text{prob. there}\\ \text{is no carrier}\\ \text{at } p}}{[1-f(p)]}\underset{\substack{\nwarrow\\ \text{transition}\\ \text{rate for the}\\ \text{collision}\\ p'\to p\\ \text{(Fermi's}\\ \text{golden rule)}}}{S(p',p)}$$

Similarly, the rate for process (2) is given by:

$$\boxed{\qquad\qquad\qquad\qquad\qquad\qquad}$$

The total rate of change at *p* due to collisions is then the sum over all possible processes scattering scattering particles into *p* minus the sum of all processes scattering particles out of *p*:

$$\left.\frac{\partial f(r,p,t)}{\partial t}\right|_{Coll} = \sum_{p'}\{f(p')[1-f(p)]S(p',p)-f(p)[1-f(p')]S(p,p')\}$$

$S(p,p')$ could be a sum of several processes.

Given $S(p,p')$, the BTE is an “integro-differential” eqn for *f (r, p, t).* (i.e. a mess!)

The name of the game is finding suitable approximations and computational techniques.

Relaxation time approximation (RTA)

Simplest approximation for the collision term:

where f_o represents the equilibrium distribution.

This simply says that equilibrium is restored in time τ. We will use this approximation heavily.

The solution then is simply:

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

Conductivity in the RTA

Assume n-type semiconductor, applied field $\vec{\mathcal{E}}$.

Further assume system is spatially uniform so that $\nabla_r f = 0$.

Steady state implies $\frac{\partial f}{\partial t} = 0$.

Then

Rewrite:

$$f = f_0 - \tau q \vec{\mathcal{E}} \cdot \vec{\nabla}_p f$$

For low field, assume small change in the momentum gradient. That is: $\vec{\nabla}_p f \cong \vec{\nabla}_p f_0$. Then:

$$f = f_o - \tau q \vec{\mathcal{E}} \cdot \vec{\nabla}_p f_o \qquad (1)$$

To improve on the first order approximation, we could iterate. That is, put this f in $\vec{\nabla}_p f$. This would give a term $O(\mathcal{E}^2)$ in the solution for f. We will neglect this for now.

Take $\vec{\mathcal{E}}$ along $\hat{z}$.

This looks like the first 2 terms of a Taylor series. Then, to 1st order: (assuming τ constant) which is the drifted Maxwellian!

We can derive another useful form. Let:

$$\theta \equiv \left[E_C - E_F + \frac{p^2}{2m^*}\right] / (kT)$$

$$f_o = e^{-\theta}$$

then

$$\vec{\nabla}_p f_o = \underbrace{\frac{\partial f_o}{\partial \theta}}_{-f_o} \underbrace{\vec{\nabla}_p \theta}_{\frac{\vec{p}}{m^* kT} = \frac{\vec{v}}{kT}}$$

Equation (1) becomes:

$$f = f_o + \frac{q\tau}{kT} f_o \vec{\mathcal{E}} \cdot \vec{v}$$

$$\equiv f_o + f' \qquad (2)$$

with $f' \ll f_o$.

Now calculate drift velocity

$$\langle v_z \rangle = \frac{\sum_p v_z (f_o + f')}{\sum_p (f_o + f')} \qquad (3)$$

If τ is constant (independent of p or E), then by inspection of drifted Maxwellian:

Current density is given by:

$$= \frac{nq^2\tau}{m^*}\mathcal{E}_z$$

$$= nq\mu\mathcal{E}_z$$

This is the familiar result with .

what if $\tau = \tau(E)$? This is the case for most scattering mechanisms.

In (3), note that f_o is even in p, f' is odd in p.
Thus:

$$\langle v_z\rangle = \frac{\sum\limits_p v_z f'}{\cancelto{n}{\sum\limits_p f_o}}$$

insert (2)

$$\langle v_z\rangle = q\mathcal{E}_z\frac{\sum\limits_p v_z^2\tau(E)f_o}{nkT}$$

$$= \frac{q}{m^*}\frac{\sum\limits_p\left(\frac{1}{2}m^*v_z^2\right)\tau(E)f_o}{\frac{1}{2}nkT}\mathcal{E}_z$$

By spherical symmetry, $v_z^2 \rightarrow \frac{1}{3}v^2$. We also know that . Incorporating these relations, we find:

$$\langle v_z\rangle = \frac{q}{m^*}\frac{\frac{1}{3}\sum\limits_p\left(\frac{1}{2}m^*v^2\right)\tau(E)f_o}{\frac{1}{3}\langle E\rangle}\mathcal{E}_z$$

$$= \frac{q}{m^*}\frac{\langle E\tau(E)\rangle}{\langle E\rangle}\mathcal{E}_z$$

If we write: $\langle v_z \rangle = \mu \mathcal{E}_z$, then this defines μ more generally:

$$\mu = \frac{q\langle\langle\tau\rangle\rangle}{m^*}.$$

This special ensemble average is defined by: $\boxed{\qquad\qquad\qquad\qquad\qquad\qquad}$.

Often $\tau(E)$ is given by a power law:

$$\tau(E) = \tau_0[E/(kT)]^s$$

Then:

$$\langle\langle\tau\rangle\rangle = \tau_0 \frac{\sum_p (p^2/2m^*)(p^2/2m^*kT)^s e^{-p^2/2m^*kT}}{\sum_p (p^2/2m^*)e^{-p^2/2m^*kT}}$$

$$= \tau_0 \frac{\int_0^\infty (p^2/2m^*kT)^s e^{-p^2/2m^*kT} p^4 dp}{\int_0^\infty e^{-p^2/2m^*kT} p^4 dp}$$

$$\text{let} \quad y \equiv p^2/2m^*kT \qquad\qquad dy = \frac{2pdp}{2m^*kT} = \frac{\sqrt{2}y^{1/2}}{(m^*kT)^{1/2}}dp$$

Then

$$\langle\langle\tau\rangle\rangle = \tau_0 \frac{\int_0^\infty y^s e^{-y} \cancel{(2m^*kT)^2} y^2 \cancel{\left(\frac{m^*kT}{2}\right)^{\frac{1}{2}}} y^{-\frac{1}{2}} dy}{\int_0^\infty e^{-y} \cancel{(2m^*kT)^2} y^2 \cancel{\left(\frac{m^*kT}{2}\right)^{\frac{1}{2}}} y^{-\frac{1}{2}} dy}$$

$$= \tau_0 \frac{\int_0^\infty y^{s+\frac{3}{2}} e^{-y} dy}{\int_0^\infty y^{\frac{3}{2}} e^{-y} dy}$$

Using the Γ function:

$\Gamma(n) = (n-1)!$ (integer n)
$\Gamma(p+1) = p\Gamma(p)$ (real p)

Finally: