coupled current equations

\[ J_x = \sigma E_x - \sigma S \frac{dT_L}{dx} \]
\[ J^q_x = T_L \sigma S E_x - \kappa_0 \frac{dT_L}{dx} \]
\[ E_x = \rho J_x + S \frac{dT_L}{dx} \]
\[ J^q_x = \pi J_x - \kappa^e_x \frac{dT}{dx} \]

(diffusive transport)

\[ \sigma = \int \sigma'(E) dE \]

\[ \sigma'(E) = \frac{2q^2}{h} \lambda(E) \frac{M(E)}{A} \left( -\frac{\partial f_0}{\partial E} \right) \]

\[ S = -\frac{k_B}{q} \int \left( \frac{E - E_F}{k_B T_L} \right) \sigma'(E) dE \left/ \int \sigma'(E) dE \right. \]

\[ \pi = T_L S \]

\[ \kappa_0 = T_L \left( \frac{k_B}{q} \right)^2 \int \left( \frac{E - E_F}{k_B T_L} \right)^2 \sigma'(E) dE \]

\[ \kappa_e = \kappa_0 - \pi S \sigma \]
goals

1) Find an equation for \( f(r, p, t) \) out of equilibrium
2) Learn how to solve it near equilibrium
3) Relate the results to our Landauer approach results – in the diffusive limit
4) Add a \( B \)-field and show how transport changes
quantum vs. semi-classical transport

\[ p = \hbar k = \hbar \frac{2\pi}{\lambda_p} \]
\[ E = \frac{p^2}{2m} = \frac{3}{2} k_B T \]
\[ \lambda_p \approx 10 \text{nm} \text{ (electrons in Si at 300K)} \]
semi-classical transport

\[ E(x, k) = E_c(x) + E(k) \]

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semi-classical transport

\[ E_{\text{TOT}} = E_c(x) + E(k) \]

\[ \frac{dE_{\text{TOT}}(x,k)}{dt} = 0 = \frac{dE_c(x)}{dx} \frac{dx}{dt} + \frac{dE(k)}{dk} \frac{dk}{dt} \]

\[ 0 = \frac{dE_c(x)}{dx} v_x + \frac{1}{\hbar} \frac{dE}{dk} \frac{dk}{dt} \frac{d}{dt} \]

\[ 0 = \frac{dE_c(x)}{dx} v_x + v_x \frac{d}{dt} \frac{d}{dt} \frac{d}{dt} = \frac{d}{dt} \frac{d}{dt} \frac{d}{dt} = F_x = - \frac{dE_c(x)}{dx} \]

---

semi-classical transport

\[ \frac{d\langle \hbar^2 \rangle}{dt} = -\nabla_r E_c(\vec{r}) = -q \vec{E}(\vec{r}) \]

\[ \left\{ \frac{d\vec{p}}{dt} = \vec{F}_e \right\} \]

\[ \hbar \dot{k}(t) = \hbar \dot{k}(0) + \int_0^t -q \vec{E}(t') dt' \]

\[ \ddot{v}_x(t) = \frac{1}{\hbar} \nabla_x E \left[ \frac{\hbar}{\hbar} \dot{k}(t) \right] \]

\[ \ddot{r}(t) = \ddot{r}(0) + \int_0^t \ddot{v}_x(t') dt' \]

equations of motion for “semi-classical transport”

\[ E_c \text{ varies slowly on the scale of the electron’s wavelength.} \]

\[ \text{no effective mass!} \]
exercise: equations of motion for $m^*(x)$

i) assume:

$$E(k,\bar{r}) = \frac{\hbar^2 k^2}{2m^*(\bar{r})}$$

ii) assume that $m^*$ varies slowly with position

iii) derive the equation of motion in $k$-space

outline

1) Introduction
2) Equation of motion
3) The BTE
4) Solving the s.s. BTE
5) Discussion
6) Summary
Boltzmann Transport Equation (BTE)

\[ T(t) = [x(t), p_x(t)] \]

\[ f(x, p_x, t) = f(x - v_x dt, p_x - F_x dt, t - dt) \]

\[ \frac{df}{dt} = 0 \]
Boltzmann Transport Equation (BTE)

\[
f(x,p_z,t) \quad \frac{df}{dt} = 0
\]

\[
\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x} \frac{dx}{dt} + \frac{\partial f}{\partial p_z} \frac{dp_z}{dt} = 0
\]

\[
\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x} v_x + \frac{\partial f}{\partial p_z} F_z = 0
\]

\[
\frac{df}{dt} + \vec{v} \cdot \nabla_r f + \vec{F}_e \cdot \nabla_p f = 0
\]

\[
\vec{F}_e = -q\vec{E} - q\vec{v} \times \vec{B}
\]

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

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

\[
\vec{p} = \hbar \vec{k}
\]

result

\[
f(\vec{r}, \vec{p}, t)
\]

\[
\frac{\partial f(\vec{r}, \vec{p}, t)}{\partial t} + \{\vec{v} \cdot \nabla_r f + \vec{F}_e \cdot \nabla_p f\} = G(\vec{r}, \vec{p}, t) - R(\vec{r}, \vec{p}, t)
\]

optical absorption, impact ionization, etc.
and carrier scattering
Boltzmann Transport Equation (BTE)

\[ \frac{df}{dt} + \bar{v} \cdot \nabla_x f + \bar{F} \cdot \nabla_v f = 0 \]

**assumptions:**

1) semi-classical treatment of electrons in a crystal with \( E(k) \)

\[
\frac{d(\hbar \vec{k})}{dt} = -\nabla E_c(\vec{r}) = -q \vec{E}(\vec{r}) \quad E = E_c(\vec{r}) + E(\vec{k})
\]

\[
\nu_s(t) = \frac{1}{\hbar} \nabla_x E \left[ k(t) \right] \quad \Delta p_x \Delta x \geq \hbar
\]

2) neglected generation-recombination

3) neglected e-e correlations (mean-field-approximation)

---

**in and out-scattering**

\[ p_x = \hbar k_x \]

\[ T(t) = [x(t), p_x(t)] \]

\[ \frac{df}{dt} \bigg|_{\text{coll}} = \hat{C}f = \text{in-scattering - out-scattering} \]

position, \( x \), does not change
scattering operator

\[ \frac{df}{dt}_{\text{coll}} = \hat{C}f(\vec{r}, \vec{p}, t) = \text{in-scattering rate} - \text{out-scattering rate} \]

in-scattering rate = \[ \sum_{\vec{p}'} S(\vec{p}' \rightarrow \vec{p}) f(\vec{p}') \left[ 1 - f(\vec{p}) \right] \]

out-scattering rate = \[ \sum_{\vec{p}'} S(\vec{p} \rightarrow \vec{p}') f(\vec{p}) \left[ 1 - f(\vec{p}') \right] \]

\[ \hat{C}f(\vec{r}, \vec{p}, t) = \sum_{\vec{p}'} S(\vec{p}' \rightarrow \vec{p}) f(\vec{p}') \left[ 1 - f(\vec{p}) \right] - \sum_{\vec{p}'} S(\vec{p} \rightarrow \vec{p}') f(\vec{p}) \left[ 1 - f(\vec{p}') \right] \]

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non-degenerate scattering operator

\[ \hat{C}f(\vec{r}, \vec{p}, t) = \sum_{\vec{p}'} S(\vec{p}' \rightarrow \vec{p}) f(\vec{p}') \left[ 1 - f(\vec{p}) \right] - \sum_{\vec{p}'} S(\vec{p} \rightarrow \vec{p}') f(\vec{p}) \left[ 1 - f(\vec{p}') \right] \]

probability that the state at \( \vec{p}' \) is occupied

probability that the state at \( \vec{p} \) is empty

\[ \hat{C}f(\vec{r}, \vec{p}, t) = \sum_{\vec{p}'} S(\vec{p}' \rightarrow \vec{p}) f(\vec{p}') - \sum_{\vec{p}'} S(\vec{p} \rightarrow \vec{p}') f(\vec{p}) \]

non-degenerate scattering operator (assumes final state empty)

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We are discussing scattering mechanisms that move carriers around in \( k \)-space. They do not create or destroy carriers.

\[
\sum_p \hat{C}f(r, \bar{p}, t) = 0
\]

\[
\sum_{p'} \left\{ \sum_{p'} S(p', \bar{p}) f(p') - \sum_{p'} S(p, \bar{p}') f(p) \right\} = \sum_{p, p'} S(p', \bar{p}) f(p') - \sum_{p, p'} S(p, \bar{p}') f(p)
\]

\[
\sum_{p, p'} S(p', \bar{p}) f(p') = \sum_{p, p'} S(p', \bar{p}) f(p') \quad \text{(interchange order of summation)}
\]

\[
\sum_{p, p'} S(p', \bar{p}) f(p') = \sum_{p, p'} S(p, \bar{p}') f(p) \quad \text{(interchange labels of dummy indices)}
\]

Relaxation Time Approximation (RTA)

\[
\hat{C}f = -\left( \frac{f(\bar{p}) - f_0(\bar{p})}{\tau_m} \right)
\]

\[
\delta f = f(\bar{p}) - f_0(\bar{p})
\]

\[
\hat{C}f = -\frac{\delta f(\bar{p})}{\tau_m}
\]

See Lundstrom: pp. 139-141. The RTA can be justified when the scattering is isotropic and/or elastic in which case the proper time to use is the "momentum relaxation time."
meaning of the RTA

\[ \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \mathbf{F}_x \cdot \nabla_p f = 0 \]
Assume spatial uniformity, no \( E \)-field.

\[ \frac{\partial f}{\partial t} = -\frac{\delta f}{\tau_m} \]
\[ \delta f = f - f_0 \]

\[ \frac{\partial (\delta f)}{\partial t} = -\frac{\delta f}{\tau_m} \]
\[ \delta f (t) = \delta f (0) e^{-t/\tau_m} \]

Perturbations decay away exponentially with a characteristic time, \( \tau_m \)

steady-state BTE in 1D

\[ \mathbf{v}_x \frac{\partial f}{\partial x} + F_x \frac{\partial f}{\partial p_x} = -\frac{\delta f}{\tau_m} \]

RTA

\[ f (\vec{p}) = f_0 (\vec{p}) + \delta f (\vec{p}) \]
\[ |f_0 (\vec{p})| >> |\delta f (\vec{p})| \]
\[ \delta f (\vec{p}) = f (\vec{p}) - f_0 (\vec{p}) \]

near-equilibrium

no B-fields for now

\[ F_x = -qE_x \]
1) Introduction
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4) **Solving the s.s. BTE**
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**near eq., s.s BTE**

\[
\mathbf{v} \cdot \nabla_r f - q\mathbf{E} \cdot \nabla_p f = -\frac{\delta f(\bar{p})}{\tau_m}
\]

\[
\mathbf{v} \cdot \nabla_r f_0 - q\mathbf{E} \cdot \nabla_p f_0 = -\frac{\delta f(\bar{p})}{\tau_m}
\]

\[
\delta f(\bar{p}) = -\tau_m \mathbf{v} \cdot \nabla_r f_0 + q\tau_m \mathbf{E} \cdot \nabla_p f_0
\]
BTE solution

\[ \delta f = -\tau_m \bar{\nu} \cdot \nabla_r f_0 + q \tau_m \bar{\Theta} \cdot \nabla_p f_0 \]

\[ f_0 (\bar{\nu}) = \frac{1}{1 + e^{\Theta}} \]

\[ \Theta (\bar{\nu}, \bar{n}) = \left[ E (\bar{r}, \bar{n}) - F_0 (\bar{r}) \right] / k_B T_L \]

\[ = \left[ E_c (\bar{r}) + E (\bar{n}) - F_0 (\bar{r}) \right] / k_B T_L \]

\[ \nabla_r f_0 = \frac{\partial f_0}{\partial \Theta} \nabla_r \Theta \]

\[ \nabla_p f_0 = \frac{\partial f_0}{\partial \Theta} \nabla_p \Theta \]

\[ \frac{\partial f_0}{\partial \Theta} = k_B T_L \frac{\partial f_0}{\partial E} \]

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BTE solution

\[ \delta f = \tau_m k_B T_L \left( -\frac{\partial f_0}{\partial E} \left[ \bar{\nu} \cdot \nabla_r \Theta - q \bar{\Theta} \cdot \nabla_p \Theta \right] \right) \]

\[ \Theta (\bar{r}, \bar{n}) = \left[ E_c (\bar{r}) + E (\bar{n}) - F_0 (\bar{r}) \right] / k_B T_L \]

\[ \nabla_r \Theta = \frac{1}{k_B T_L} \left[ \nabla_r E_c - \nabla_r F_0 \right] + \left[ E_c + E (\bar{n}) - F_0 \right] \nabla_r \left( \frac{1}{k_B T_L} \right) \]

\[ \nabla_p \Theta = \frac{\bar{\nu} (\bar{n})}{k_B T_L} \]

\[ \delta f = \tau_m \left( -\frac{\partial f_0}{\partial E} \right) \bar{\nu} \cdot \left( -\nabla_r F_0 + T_L \left[ E_c + E (\bar{n}) - F_0 \right] \nabla_r \left( \frac{1}{T_L} \right) \right) \]

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The two forces driving current flow are gradients in QFL and gradients in (inverse) temperature. In Lecture 4, we saw that \((f_1 - f_2)\) produces current flow and that differences in Fermi level and temperature cause differences in \(f\).
another look at the solution…

\[ \delta f = \tau_m \left( -\frac{\partial f}{\partial E} \right) \vec{v} \rightarrow \tau_m \left( -\frac{\partial f}{\partial E} \right) v_x \vec{F}_x \]

\[ \vec{F} = -\nabla F_n + T_L \left[ E_c + E(k) - F_n \right] \nabla r \left( \frac{1}{T_L} \right) \rightarrow -\frac{dF_n}{dx} = -qE_x \]

\[ \delta f = q \tau_m E_x \left( \frac{\partial f_0}{\partial E} \right) v_x \]

\[ q \tau_m E_x \left( \frac{\partial f_0}{\partial p_x} \right) \left( \frac{\partial p_x}{\partial E} \right) v_x = q \tau_m E_x \left( \frac{\partial f_0}{\partial p_x} \right) \]

another look at the solution…

\[ \delta f = \left( \frac{\partial f_0}{\partial p_x} \right) q \tau_m E_x \]

\[ f = f_0 + \delta f = f_0 + \left( \frac{\partial f_0}{\partial p_x} \right) q \tau_m E_x \]

Recall:

\[ g(x+dx) = g(x) + \frac{\partial g}{\partial x} dx + \ldots \]

\[ f(\vec{p}) = f_0 (\vec{p} + dp_x \hat{x}) \]

\[ dp_x = q \tau_m E_x \]

So the distribution has been displaced by \( p_d \) is a directionopposite to the electric field

\[ \delta p_x = -q \tau_0 E_x \]

\[ \tau_m = \tau_0 \]
now what?

\[ \delta f = \tau_m \left( -\frac{\partial f}{\partial E} \right) \bar{v} \cdot \mathbf{F} \]

We have solved the BTE, now what do we do with the solution?

**moments**

\[ n(\mathbf{r}) = \frac{1}{\Omega} \sum_k f_0(\mathbf{r}, \mathbf{k}) + \delta f(\mathbf{r}, \mathbf{k}) = \frac{1}{\Omega} \sum_k f_0(\mathbf{r}, \mathbf{k}) \]

\[ \mathbf{J}_a(\mathbf{r}) = \frac{1}{A} \sum_k (-g) \bar{u}(\mathbf{k}) \delta f(\mathbf{r}, \mathbf{k}) \]

\[ \mathbf{J}_w(\mathbf{r}) = \frac{1}{A} \sum_k E(\mathbf{k}) \bar{u}(\mathbf{k}) \delta f(\mathbf{r}, \mathbf{k}) \]

\[ \mathbf{J}_q(\mathbf{r}) = \frac{1}{A} \sum_k \left( E(\mathbf{k}) - F \right) \bar{u}(\mathbf{k}) \delta f(\mathbf{r}, \mathbf{k}) \]

To evaluate these quantities, we need to work out sums in \( k \)-space.
moments

\[ n(\mathbf{r}) = \frac{1}{\Omega} \sum_k f_0(\mathbf{r}, \mathbf{k}) + \delta f(\mathbf{r}, \mathbf{k}) = \frac{1}{\Omega} \sum_k f_0(\mathbf{r}, \mathbf{k}) \]

\[ \mathbf{J}_n(\mathbf{r}) = \frac{1}{A} \sum_k (-q)\mathbf{v}(\mathbf{k})\delta f(\mathbf{r}, \mathbf{k}) \]

\[ \mathbf{J}_w(\mathbf{r}) = \frac{1}{A} \sum_k E(\mathbf{k})\mathbf{v}(\mathbf{k})\delta f(\mathbf{r}, \mathbf{k}) \]

\[ \mathbf{J}_Q(\mathbf{r}) = \frac{1}{A} \sum_k (E(\mathbf{k}) - F_n)\mathbf{v}(\mathbf{k})\delta f(\mathbf{r}, \mathbf{k}) \]

To evaluate these quantities, we need to work out sums in \( k \)-space.

recall lecture 4

outline

1) Introduction
2) Equation of motion
3) The BTE
4) Solving the s.s. BTE
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summary

1) Semi-classical transport assumes a bulk bandstructure with a slowly varying applied potential.

2) Semiclassical transport ignores quantum reflections and assumes that position and momentum can both be precisely specified.

3) The Boltzmann Transport Equation can be solved to find the probability that states in the device are occupied.

4) In equilibrium, the solution to the BTE is the Fermi function.

BTE:
\[
\frac{\partial f}{\partial t} + \bar{\nu} \cdot \nabla f + \bar{F}_e \cdot \nabla_p f = \hat{C} f \\
\hat{C} f (\bar{r}, \bar{p}, t) = \sum_{\rho'} S(\rho', \bar{p}) f(\rho') [1 - f(\bar{p})] - \sum_{\rho'} S(\rho, \bar{p}') f(\rho) [1 - f(\rho')] 
\]

RTA:
\[
\hat{C} f = -(f(\bar{p}) - f_0(\bar{p})) / \tau_m 
\]

Solution:
\[
\delta f = \tau_m \left( -\frac{\partial f_0}{\partial E} \right) \bar{\nu} \cdot \bar{F} \\
\bar{F} = - \nabla \cdot F_n + T_L \left[ E_c + E(k) - F_n \right] \nabla \left( \frac{1}{T_L} \right) 
\]
questions

1) Introduction
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