ECE-656: Fall 2009

Lecture 12: Boltzmann Transport Equation

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\[ f(r, k, t) \]

\[
f(x, k_x, t) = \frac{1}{1 + e^{(E - E_F)/k_B T}}
\]
finding \( f(r, k, t) \): by analogy

\[
\frac{\partial n}{\partial t} = -\nabla \cdot \frac{J_n}{(-q)} + G_n - R_n
\]

\[
\frac{r}{J_n} = qn \langle \nu \rangle = qn \left< \frac{dr}{dt} \right>
\]

\[
\frac{\partial f}{\partial t} = -\nabla g(\nu f) + (G - R)
\]

\[
\frac{r}{J} = f\left( \frac{dr}{dt} + \frac{1}{h} \frac{dk}{dt} \right)
\]

\[
\nabla g \frac{r}{f} = \nabla_r g \left( \nu f \right) + \nabla_k g \left( \frac{1}{h} \frac{dk}{dt} f \right)
\]

\[
= \nu g \nabla_r f + \nabla_k g \left( \frac{1}{h} \frac{dk}{dt} f \right)
\]

\[
h \frac{dk}{dt} = \frac{r}{F_e} = -qE
\]

\[
(G - R) = \frac{df}{dt}\bigg|_{\text{coll}} + \frac{df}{dt}\bigg|_{\text{other}}
\]

\[
\frac{\partial f}{\partial t} = -r \nu g \nabla_r f - \frac{1}{h} \frac{r}{F_e} \cdot \nabla_k f + \frac{df}{dt}\bigg|_{\text{coll}}
\]
1) Introduction
2) Semi-classical electron dynamics
3) Boltzmann Transport Equation (BTE)
4) Scattering
5) Discussion
6) Summary
quantum vs. semi-classical

particle or wave?

\[ p = \hbar k = \hbar \frac{2\pi}{\lambda_B} \]

\[ E = \frac{p^2}{2m^*} \approx \frac{3}{2} k_B T \]

\[ \lambda_B = \sqrt{\frac{4\pi^2\hbar^2}{3m^* k_B T}} \]

particle when \( E_C(x) \) varies slowly on the scale of the electron’s wavelength

\( p \approx \frac{h}{e} \frac{2\pi}{\lambda_B} \approx \frac{3}{2} k_B T \) for electrons in Si at 300K.
semi-classical transport

\[ E(x, k) = E_C(x) + E(k) \]
semi-classical transport

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

\[ k_1 > k_0 \]

“free flight” (followed by scattering)
semi-classical transport

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

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

\[
0 = \frac{dE_C(x)}{dx} \nu_x + \frac{1}{h} \frac{dE}{dk_x} \frac{d(hk_x)}{dt}
\]

\[
0 = \frac{dE_C(x)}{dx} \nu_x + \nu_x \frac{d(hk_x)}{dt}
\]

\[
\frac{d(hk_x)}{dt} = F_e = -\frac{dE_C(x)}{dx}
\]
semi-classical transport

\[ \frac{d(hk)}{dt} = -\nabla_r E(r) = -q\mathcal{E}(r) \]
\[ \left\{ \frac{dp}{dt} = F_e \right\} \]

\[ \begin{aligned}
    r_k(t) &= r_k(0) + \int_0^t -q\mathcal{E}(t') \, dt' \\
    \tilde{\nu}_g(t) &= \frac{1}{\hbar} \nabla_k E \left[ k(t) \right] \\
    \tilde{r}(t) &= r(0) + \int_0^t \tilde{\nu}_g(t') \, dt'
\end{aligned} \]

equations of motion for semi-classical transport
exercise: equations of motion when $m^*(x)$

i) assume:

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

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

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

\[ p_x = \hbar k_x \]

\[ h k_x (t) = h k_x (0) + \int_0^t -q E_x (t') dt' \]

\[ x(t) = x(0) + \int_0^t v_x (t') dt' \quad v_x (t) = \frac{d E}{d (h k_x)} \bigg|_{k(t)} \]

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

\[ \left\{ \mathcal{E} (x, t) = \mathcal{E}_x (x, t) \hat{x} \right\} \]
Boltzmann Transport Equation (BTE)

\[ p_x = \hbar k_x \]

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

\[ f(x, p_x, t) = f(x - \nu_x dt, p_x - F_e dt, t - dt) \]

\[ \frac{df}{dt} = 0 \]
The Boltzmann Transport Equation (BTE) is given by:

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

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

\[ \frac{df}{dt} = \frac{\partial f}{\partial t} + \nu_x \frac{\partial f}{\partial x} + \frac{\partial f}{\partial p_x} F_x = 0 \]

\[ \frac{\partial f}{\partial t} + \nu \cdot \nabla_r f + \mathbf{F}_e \cdot \nabla_p f = 0 \]

Where:

\[ \mathbf{F}_e = -qE - q\mathbf{v} \times \mathbf{B} \]

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

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

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

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another view: continuity equation

\[
p(r, t) \cdot \nabla \left( \frac{J_p}{q} \right) = \frac{\partial p(r, t)}{\partial t} + G(r, t) - R(r, t)
\]
continuity equation view

\[ f(r, p, t) \]

\[-\nabla \cdot \left[ \left( \nu_x \dot{x} f + \nu_{p_x} \dot{p}_x f \right) \right] = \frac{\partial f(x, p_x, t)}{\partial t} + G(x, p_x, t) - R(x, p_x, t)\]

**Exercise:** work out the details and show that we get the same BTE.
result

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

\[
\frac{\partial f(x, p_x, t)}{\partial t} + \left\{ \mathbf{v} \cdot \nabla \mathbf{r} f + \mathbf{F}_e \cdot \nabla \mathbf{p} f \right\} = G(\mathbf{r}, \mathbf{p}, t) - R(\mathbf{r}, \mathbf{p}, t)
\]

optical absorption, impact ionization, etc.
and carrier scattering
1) Introduction
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carrier scattering

\[ p_x = \hbar k_x \]

\[ \frac{df}{dt} \neq 0 \]

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

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

“in-scattering”

“out-scattering”
Boltzmann Transport Equation (BTE)

\[ \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f + F_e \cdot \nabla_{\mathbf{p}} f = \hat{C} f \]

\[ f(r, p, t) \]

**assumptions:**

1) semi-classical treatment of electrons:

\[ \frac{d(h\mathcal{k})}{dt} = -\nabla E_C(r) = -qE(r) \quad E = E_C(r) + E(k) \quad \Delta p_x \Delta x \geq h \]

2) neglected generation-recombination

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

\[ p_x = \hbar k_x \]

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

"in-scattering" \hspace{1cm} "out-scattering"

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

\[ p_x = \hbar k_x \]

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

\[ f(x, p_x, t) \]

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

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

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

in-scattering rate = \(\sum_{p'} S(p', p) f(p') [1 - f(p)]\)

out-scattering rate = \(\sum_{p'} S(p, p') f(p) [1 - f(p')]\)

\[
\hat{C}f(r, p, t) = \sum_{p'} S(p', p) f(p') [1 - f(p)] - \sum_{p'} S(p, p') f(p) [1 - f(p')]
\]
non-degenerate scattering operator

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

- probability that the state at \( p' \) is occupied
- probability that the state at \( p \) is empty

non-degenerate scattering operator
(assumes final state empty)
conservation of carriers

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

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

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

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

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

\[ \vec{p}_0 = \hbar k \]

\[ S(p, p') \]

Transition rate: Probability per unit time that a carrier with momentum, $p$, makes a transition to $p'$ (assuming that $p$ is occupied and that $p'$ is empty).

\[ S(p_0, p') f(p_0) [1 - f(p')] \]

Actual rate of transitions

1) Identify scattering potential

2) Compute transition rate quantum mechanically (typically using Fermi’s Golden Rule)
outline

1) Introduction
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the BTE

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

\[
\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{r}} f + \mathbf{F}_e \cdot \nabla_p f =\\
\]

\[
\sum_{p'} S(\mathbf{r}', p') f(\mathbf{r}') [1 - f(\mathbf{r})] - \sum_{p'} S(\mathbf{r}, p') f(\mathbf{r}) [1 - f(\mathbf{r}')]
\]

Six-dimensional integro-differential equation for \( f(r, p, t) \).
solving the BTE

(x, y, z) 3 independent variables
(k_x, k_y, k_z) 3 more independent variables
+ time..... 7 dimensional

(100 x 100 x 100) x (100 x 100 x 100) x 10 = 10^{13} unknowns!
“curse of dimensionality”

A difficult problem ... We will need to make approximations in order to solve the BTE.
using $f(x, k_x, t)$

\[ n(x,t) = \frac{1}{\Omega} \int_{-\infty}^{\infty} f(x,k,t) N_k \, d^3k \]

\[ J(x,t) = \frac{1}{\Omega} \int_{-\infty}^{\infty} (-q) \nu_x(k) \times f(x,k,t) N_k \, d^3k \]

\[ P_x(x,t) = \frac{1}{\Omega} \int_{-\infty}^{\infty} m^* \nu(k) \times f(x,k,t) N_k \, d^3k \]

\[ W(x,t) = \frac{1}{\Omega} \int_{-\infty}^{\infty} (E - E_C) \times f(x,k,t) N_k \, d^3k \]

....
assumptions

1) Semi-classical treatment of electrons:
   Electrons respond semi-classically to the local electric field. Quantum transport models (like the NEGF approach) remove this assumption.

2) Neglected generation-recombination:
   But can add for specific problems (e.g. photoexcitation, impact ionization, etc).

3) Neglected e-e correlations
   So-called ensemble Monte Carlo (or molecular dynamics) simulations can treat these many body effects.
Outline

1) Introduction
2) Semiclassical electron dynamics
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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.
questions

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