6.730 Physics for Solid State Applications

Lecture 33: Boltzman Equations: Moments of

Outline

- Last Time: Boltzmann Transport Equation
- Introduction to Balance Equations
  - Moments of BTE

April 30, 2004

Scattering Rate Calculations

Overview

Step 1: Determine Scattering Potential

$$U_S(r,t) = U^a(r)e^{-i\omega t} + U^e(r)e^{+i\omega t}$$

Step 2: Calculate Matrix Elements

$$H^a_{k'k} = \int_V \psi_{nk'}(r)\; U^a_s(r)\; \psi_{nk}(r)\; d^3r$$

Step 3: Calculate State-State Transition Rates

$$S(k,k') = \frac{2\pi}{\hbar}\left[|H^a_{k'k}|^2\delta(E(k')-E(k)-\hbar\omega) + |H^e_{k'k}|^2\delta(E(k')-E(k)+\hbar\omega)\right]$$

Step 4: Calculate State Lifetime

$$\frac{1}{\tau(k)} = \sum_{k'} S(k,k')\left(1-f(k')\right)$$

Step 5: Calculate Ensemble Lifetime

$$<\tau>$$

Properties of the Occupancy Function

Moments of *f* (*r,k,t*)

Carrier density...

$$n(r,t) = \frac{1}{V} \sum_k f(r,k,t)$$

Current density...

$$J(r,t) = \frac{-q}{V} \sum_k \nabla_k E(k)\, f(r,k,t)$$

$$\approx \frac{-q}{V} \sum_k \frac{\hbar k}{2m^*} f(r,k,t)$$

Energy density...

$$W(r,t) = \frac{1}{V} \sum_k E(k)\, f(r,k,t)$$

$$\approx \frac{1}{V} \sum_k \frac{\hbar^2 k^2}{2m^*} f(r,k,t)$$

All the classical information about the carriers is contained in *f* (*r,k,t*)

Rate Equations for Occupancy Function

$$\frac{df(r,k,t)}{dt} = \sum_{k'} \Big(f(k')(1 - f(k))\, S(k',k) - f(k)(1 - f(k')\, S(k,k') \Big)$$

$S(k',k)$ rate of scattering from k' to k

$S(k,k')$ rate of scattering from k to k'

Perturbations that cause scattering....

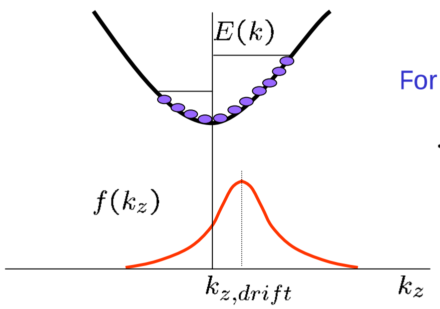
- Impurities or defects
- Electron-phonon scattering
- Electron-photon scattering

Use Fermi's Golden Rule to calculate scattering between Bloch functions...

Solving Boltzmann Transport Equation

$$\frac{\partial f}{\partial t} + \frac{\hbar \bar{k}}{m^*} \cdot \bar{\nabla}_r f + \frac{\bar{F}}{\hbar} \cdot \nabla_k f = \sum_{k'} f(k') S(k', k) - \sum_{k'} f(k) S(k, k')$$

- Usually solve BTE numerically or under the relaxation time approximation (RTA)



For low-field transport...

$$f(k) = f_S(k) + f_A(k) \approx f_o(k) + f_A(k)$$

Resistor Example

BTE Solution under RTA

$$\frac{\partial f}{\partial t} + \frac{\hbar}{m^*} \bar{k} \cdot \bar{\nabla}_r f + \frac{\bar{F}}{\hbar} \nabla_k f = -\frac{f_A}{\tau(k)} \approx \frac{-(f - f_0)}{\tau(k)}$$

For steady-state transport under a uniform electric field....

$$\Rightarrow \frac{\partial f}{\partial t} = 0 \qquad \Rightarrow \bar{\nabla}_r f = 0$$

For low field transport....

$$f = f_s + f_A \qquad \Rightarrow f_A \ll f_s \qquad \Rightarrow f_s \approx f_0$$

BTE reduces to... $\frac{-q}{\hbar} E_z \frac{\partial f_o}{\partial k_z} = \frac{-f_A}{\tau(k)}$ ⟹ $f_A = \tau(k) \frac{q}{\hbar} E_z \frac{\partial f_0}{\partial k_z}$

Resistor Example

BTE Solution under RTA

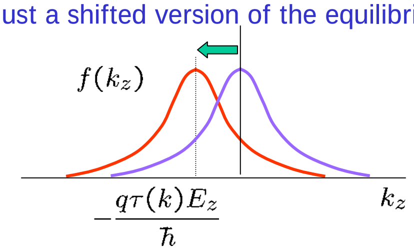
$$f = f_s + f_A$$

$$f(r,k) \approx f_0(r,k) \, + \, \tau(k) \, \frac{q}{\hbar} \, E_z \, \frac{\partial f_0(r,k)}{\partial k_z}$$

Can equate this to the Taylor Series Expansion of shifted occupancy function…

$$f_0\left(r, k_x, k_y, k_z + \frac{q\tau(k)\, E_z}{\hbar}\right) \approx f_0(r, k_x, k_y, k_z) + \left(\frac{q\tau(k)\, E_z}{\hbar}\right) \frac{\partial f_0}{\partial k_z}\Big|_{eq.}$$

So, BTE solution is just a shifted version of the equilibrium occupancy….



Relaxation Time Approximation

For isotropic scattering, RTA is exact….

- LA deformation potential scattering
- Highly screened impurity (δ-function potential)

For elastic scattering, RTA is valid for low-field transport…

- Impurity or defect scattering (Coulomb potential)
- Low energy LA deformation potential scattering is nearly elastic

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Mean of BTE

Zero Moment

$$\frac{1}{V}\sum_k \left[\frac{\partial f}{\partial t} + \frac{\hbar \overline{k}}{m^*} \cdot \overline{\nabla}_r f + \frac{\overline{F}}{\hbar} \cdot \nabla_k f = \sum_{k'} f(k')S(k',k) - \sum_{k'} f(k)S(k,k')\right]$$

$$\frac{1}{V}\sum_k \frac{\partial f}{\partial t} = \frac{\partial}{\partial t}\left(\frac{1}{V}\sum_k f(k)\right) = \frac{\partial n}{\partial t}$$

$$\frac{1}{V}\sum_k \frac{\hbar}{m^*} k \cdot \nabla_r f = \nabla_r \cdot \left(\frac{1}{V}\sum_k \frac{\hbar k}{m^*} f(k)\right) = -\frac{1}{q}\nabla_r J$$

Mean of BTE

Zero Moment

$$\frac{1}{V}\sum_k\left[\frac{\partial f}{\partial t}+\frac{\hbar\overline{k}}{m^*}\cdot\overline{\nabla}_r f+\frac{\overline{F}}{\hbar}\cdot\nabla_k f=\sum_{k'}f(k')S(k',k)-\sum_{k'}f(k)S(k,k')\right]$$

$$\frac{1}{V}\sum_k\frac{F}{\hbar}\nabla_k f=\frac{F}{\hbar}\left(\frac{1}{V}\sum_k\nabla_k f\right)\sim\frac{F}{\hbar}\left(\int_{\infty}^{\infty}\nabla_k f dk\right)$$

$$\sim\frac{F}{\hbar}\left(f(k\to\infty)-f(k\to-\infty)\right)=0$$

Mean of BTE

Zero Moment

$$\frac{1}{V}\sum_k\left[\frac{\partial f}{\partial t}+\frac{\hbar\overline{k}}{m^*}\cdot\overline{\nabla}_r f+\frac{\overline{F}}{\hbar}\cdot\nabla_k f=\sum_{k'}f(k')S(k',k)-\sum_{k'}f(k)S(k,k')\right]$$

$$\frac{1}{V}\sum_k\sum_{k'}\left(S(k',k)f(k')-S(k,k')f(k)\right)_{intraband}=0$$

$$\frac{1}{V}\sum_k\sum_{k'}\left(S(k',k)f(k')-S(k,k')f(k)\right)_{interband}=G-R$$

Mean of BTE

Zero Moment

$$\frac{1}{V}\sum_k \left[\frac{\partial f}{\partial t} + \frac{\hbar \overline{k}}{m^*}\cdot \overline{\nabla}_r f + \frac{\overline{F}}{\hbar}\cdot \nabla_k f = \sum_{k'} f(k')S(k',k) - \sum_{k'} f(k)S(k,k')\right]$$

$$\frac{\partial n}{\partial t} - \frac{1}{q}\nabla_r J + 0 = G - R$$

Mean of BTE is the continuity equation...
....no approximations for classical particles

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla_r J + G - R$$

Every moment of BTE generates new transport equation...

Zero-moment:
- Continuity equation

$$\frac{1}{V}\sum_k \left[\frac{\partial f}{\partial t} + \frac{\hbar \overline{k}}{m^*}\cdot \overline{\nabla}_r f + \frac{\overline{F}}{\hbar}\cdot \nabla_k f = \sum_{k'} f(k')S(k',k) - \sum_{k'} f(k)S(k,k')\right]$$

First-moment:
- Navier-Stokes equation (for fluids)
- Drift-diffusion equation

$$\frac{1}{V}\sum_k \frac{\hbar k_z}{m^*}\left[\frac{\partial f}{\partial t} + \frac{\hbar \overline{k}}{m^*}\cdot \overline{\nabla}_r f + \frac{\overline{F}}{\hbar}\cdot \nabla_k f = \sum_{k'} f(k')S(k',k) - \sum_{k'} f(k)S(k,k')\right]$$

Second-moment:
- Thermal transport

Momentum Balance Equation from BTE

First Moment

$$\frac{1}{V}\sum_k \frac{\hbar k_z}{m^*}\left[\frac{\partial f}{\partial t} + \frac{\hbar \overline{k}}{m^*}\cdot \overline{\nabla}_r f + \frac{\overline{F}}{\hbar}\cdot \nabla_k f = \sum_{k'} f(k')S(k',k) - \sum_{k'} f(k)S(k,k')\right]$$

$$\frac{1}{V}\sum_k \frac{\hbar k_z}{m^*}\frac{\partial f}{\partial t} = \frac{\partial}{\partial t}\left(\frac{1}{V}\sum_k \frac{\hbar k_z}{m^*} f(k)\right) = -\frac{1}{q}\frac{\partial J_z}{\partial t}$$

$$\frac{1}{V}\sum_k \frac{\hbar k_z}{m^*}\frac{\hbar k_i}{m^*}\frac{\partial f}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{1}{V}\sum_k \frac{\hbar^2 k_z k_i}{m^{*2}} f(k)\right) = 2\frac{1}{m^*}\frac{\partial W_{zi}}{\partial x_i}$$

$$W_{ij} = \frac{\hbar^2 k_i k_j}{2m^*}$$

Momentum Balance Equation from BTE

First Moment

$$\frac{1}{V}\sum_k \frac{\hbar k_z}{m^*}\left[\frac{\partial f}{\partial t} + \frac{\hbar \overline{k}}{m^*}\cdot \overline{\nabla}_r f + \frac{\overline{F}}{\hbar}\cdot \nabla_k f = \sum_{k'} f(k')S(k',k) - \sum_{k'} f(k)S(k,k')\right]$$

$$\frac{1}{V}\sum_k \frac{\hbar k_z}{m^*}\frac{F_z}{\hbar}\frac{\partial f}{\partial k_z} = \frac{F_z}{m^*}\left(\frac{1}{V}\sum_k k_z \frac{\partial f}{\partial k_z}\right) = \frac{F_z}{m^*}\left(\frac{1}{V}\sum_k \frac{\partial (k_z f)}{\partial k_z} - \frac{1}{V}\sum_k f\frac{\partial k_z}{\partial k_z}\right)$$

$$= \frac{F_z}{m^*}\left(\frac{1}{V}(k_z f)|_{-\infty}^{\infty} - n\right) = -\frac{nF_z}{m^*}$$

Momentum Balance Equation from BTE

First Moment

$$\frac{1}{V}\sum_k\sum_{k'}\frac{\hbar k_z}{m^*}\left(S(k',k)f(k')-S(k,k')f(k)\right)$$

$$=\frac{\hbar}{m^*}\frac{1}{V}\left(\sum_k\sum_{k'}k_zS(k',k)f(k')-\sum_k\sum_{k'}k_zS(k,k')f(k)\right)$$

$$=\frac{\hbar}{m^*}\frac{1}{V}\left(\sum_k\sum_{k'}k'_zS(k,k')f(k)-\sum_k\sum_{k'}k_zS(k,k')f(k)\right)$$

$$=-\frac{\hbar}{m^*}\frac{1}{V}\sum_k\sum_{k'}k_zS(k,k')f(k)\left(1-\frac{k'_z}{k_z}\right)$$

$$=-\frac{\hbar}{m^*}\frac{1}{V}\sum_k k_zf(k)\sum_{k'}S(k,k')\left(1-\frac{k'_z}{k_z}\right)$$

$$=-\frac{\hbar}{m^*}\frac{1}{V}\sum_k k_zf(k)\frac{1}{\tau_m(k)}\equiv\frac{J_z}{q}\langle\langle\frac{1}{\tau_m(k)}\rangle\rangle$$

Momentum Balance Equation from BTE

First Moment

$$\frac{1}{V}\sum_k\frac{\hbar k_z}{m^*}\left[\frac{\partial f}{\partial t}+\frac{\hbar\overline{k}}{m^*}\cdot\overline{\nabla}_rf+\frac{\overline{F}}{\hbar}\cdot\nabla_kf=\sum_{k'}f(k')S(k',k)-\sum_{k'}f(k)S(k,k')\right]$$

$$-\frac{1}{q}\frac{\partial J_z}{\partial t}+\frac{2}{m^*}\frac{\partial W_{zi}}{\partial x_i}-\frac{nF_z}{m^*}=J_z\langle\langle\frac{1}{\tau_m}\rangle\rangle$$

Generalized Drift-Diffusion (1-D)...

$$\frac{\partial J_z}{\partial t}=\frac{2q}{m^*}\frac{\partial W_{zi}}{\partial x_i}-\frac{nqF_z}{m^*}-J_z\langle\langle\frac{1}{\tau_m}\rangle\rangle$$

Generalized Drift-Diffusion (3-D)...

$$\frac{\partial\overline{J}}{\partial t}=\frac{2q}{m^*}\nabla_r\overline{\overline{W}}-\frac{nq\overline{F}}{m^*}-\overline{J}\langle\langle\frac{1}{\tau_m}\rangle\rangle$$

No approximations (except electron dispersion)...
works for ballistic transport & high field transport