6.730 Physics for Solid State Applications

Lecture 32: Introduction to Boltzmann Transport

Outline

- Non-equilibrium Occupancy Functions
- Boltzmann Transport Equation
- Relaxation Time Approximation Overview
- Example: Low-field Transport in a Resistor

April 28,2004

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

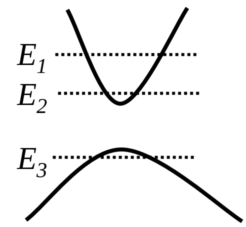
$$\frac{1}{\tau(k)} = \sum_{k'} S(k,k')\left(1 - f(k')\right)$$

Step 5: Calculate Ensemble Lifetime

$$< \tau >$$

Occupancy Functions and Quasi-Fermi Functions

$$f(E) \quad vs. \quad f(k)$$
$$f(E,r) \qquad f(k,r)$$
$$f(E,r,t) \qquad f(k,r,t)$$



Equilibrium occupancy function...

$$f_o(k,r) = \frac{1}{1 + e^{(E_c(r,k) - E_{F_o})/k_BT}}$$

Quasi-equilibrium occupancy function...

$$f(k,r) \approx \frac{1}{1 + e^{(E_c(r,k) - E_{F_c}(r))/k_BT}}$$

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...

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

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

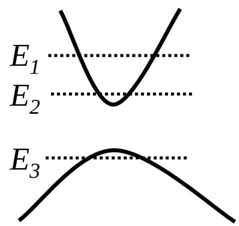
All the classical information about the carriers is contained in $f(r,k,t)$

Rate Equations for Occupancy Function

Previously we developed rate equation for model 3-level system...

$$N_2 \frac{df_2}{dt} = +k_{12} N_1 N_2 \left[f_1 (1 - f_2) - A_{12} f_2 (1 - f_1) \right]$$

$$-k_{23} N_2 N_3 \left[f_2 (1 - f_3) + A_{23} f_3 (1 - f_2) \right]$$



Now, generalize for the whole occupancy function...

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

Rate Equations for Occupancy Function

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

$S(k',k)$ 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

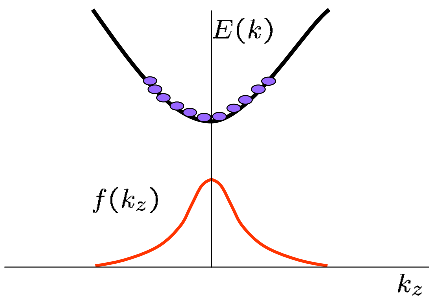
Use Fermi's Golden Rule to calculate scattering between Bloch functions...

Last Look at Equilibrium Occupancy Functions

$$f(r,k) = \frac{1}{1 + e^{[E(k)+E_c(r)-E_f]/k_B T_L}}$$

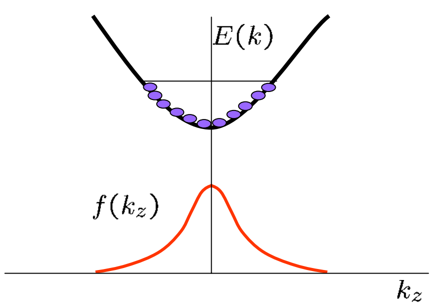
$$\approx e^{-[E(k)+E_c(r)-E_f]/k_B T_L} \quad \text{(Boltzmann Limit)}$$

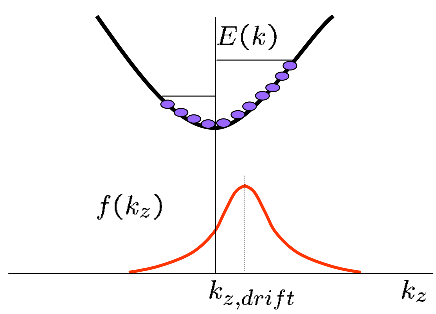
$$\approx e^{(E_f - E_c(r))/k_B T_L} \; e^{-\hbar^2 k^2 / 2m^* k_B T_L}$$



$\Rightarrow standard\ dev \sim T_e = T_L$

Intuition for Non-equilibrium Occupancy Functions





Out of equilibrium it is possible to get current....
....there are more electrons at $+k_z$ than $-k_z$

Boltzmann Transport Equation

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

1-D

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

Inserting semi-classical equations of motion...

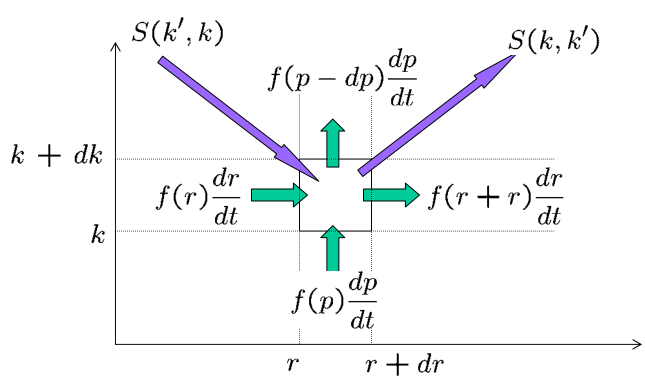
$$\Rightarrow \frac{\partial f}{\partial t} + \frac{\partial f}{\partial r} \cdot \frac{\hbar k}{m^*} + \frac{\partial f}{\partial k}\frac{F}{\hbar} = \sum_{k'} \Big(f(k')S(k',k) - f(k)S(k,k') \Big)$$

3-D

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

Boltzmann Transport Equation

Boltzmann Transport Equation



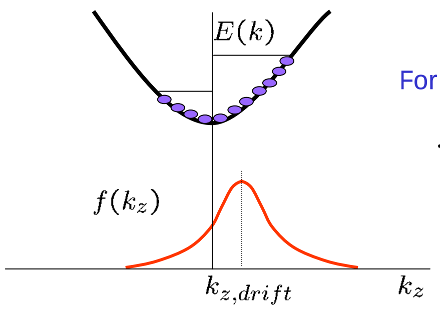
Boltzmann Transport Equation is a continuity equation for *f* (r,k,t)...

$$\frac{\partial f}{\partial t} = -\frac{\partial r}{\partial t}\frac{\partial f}{\partial r} - \frac{\partial k}{\partial t}\frac{\partial f}{\partial k} + \sum_{k'} f(k')S(k',k) - \sum_{k'} f(k)S(k,k')$$

Solving Boltzmann Transport Equation

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

- Usually solve BTE numerically or under the relaxation time approximation (RTA)
- We will derive RTA next time, today lets see what it is and how it is used...



For low-field transport...

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

Relaxation Time Approximation

$$\sum_{k'} \left(f(k') S(k', k) - f(k) S(k, k') \right)$$

$$= \sum_{k'} \left(f_S(k') S(k', k) - f_S(k) S(k, k') \right) + \sum_{k'} \left(f_A(k') S(k', k) - f_A(k) S(k, k') \right)$$

For low-field transport... $f_S(k) \approx f_o(k)$

$$\approx \sum_{k'} \left(f_A(k') S(k', k) - f_A(k) S(k, k') \right)$$

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

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

$$= -\frac{f_A(k)}{\tau(k)}$$

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....

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

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

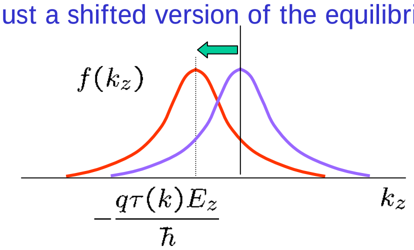
$$f = f_s + f_A$$

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

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....



Resistor Example

BTE Solution under RTA

$$J_z = -qn < v_z > = \frac{-q}{V} \sum_k \frac{\hbar k_z}{m^*} f(r,k)$$

$$J_z = \frac{-q}{V} \sum_k \left(\cancel{\frac{\hbar k_z}{m^*} f_S(r,k)} + \frac{\hbar k_z}{m^*} f_A(r,k) \right)$$

$$J_z = \frac{-q}{V} \sum_k \frac{\hbar k_z}{m^*} f_A(r,k)$$

$$< v_z > = \frac{\sum_k \frac{\hbar k_z}{m^*} f_A(r,k)}{\sum_k f_0(r,k)} \approx \frac{1}{n} \sum_k \frac{\hbar k_z}{m^*} \frac{\tau(k) q E_z}{\hbar} \frac{\partial f_0(r,k)}{\partial k_z}$$

$$= \frac{1}{n} \sum_k \frac{k_z \tau(k) q E_z}{m^*} \frac{\partial f_0(r,k)}{\partial k_z}$$

Resistor Example

BTE Solution under RTA

$$f_o(r,k) = e^{(E_F - E_c)/k_B T_L} \; e^{-\hbar^2 k^2 / 2m^* k_B T_L}$$

$$\frac{\partial f_o}{\partial k_z} = e^{(E_F - E_c)/k_B T_L} \left(\frac{-\hbar^2 k_z}{m^* k_B T_L} \right) e^{-\hbar^2 k^2 / 2m^* k_B T_L}$$

$$\frac{\partial f_o}{\partial k_z} = f_o(r,k) \left(\frac{-\hbar^2 k_z}{m^* k_B T_L} \right)$$

$$< v_z > = \frac{1}{n} \sum_k \frac{k_z \tau(k) q E_z}{m^*} \frac{\partial f_o(r,k)}{\partial k_z}$$

$$= \frac{1}{n} \sum_k \left(\frac{k_z^2 \tau(k) q E_z \; (-\hbar^2)}{m^{*2} k_B T_L} \right) f_o(r,k)$$

Resistor Example

BTE Solution under RTA

$$< v_z > = \frac{1}{n} \sum_k \left(\frac{k_z^2 \tau(k) q\, E_z \ (-\hbar^2)}{m^{*2} k_B T_L} \right) f_o(r,k)$$

$$= \frac{1}{n} \sum_k \left(\frac{\frac{-2}{3} \frac{\hbar^2 k^2}{2m^*} \tau(k) \frac{q\, E_z}{m^*}}{k_B T_L} \right) f_o(r,k)$$

$$= \frac{-\sum_k \frac{\hbar^2 k^2}{2m^*} \tau(k) \frac{q\, E_z}{m^*} f_o(r,k)}{< E >}$$

$$= \frac{-q\, E_z}{m^*} \frac{< E\tau(E) >}{< E >}$$

$$\equiv -E_z \mu_n$$

$$\Rightarrow \mu_n = \frac{< E\tau(E) >}{< E >} \frac{q}{m^*}$$

Resistor Example

BTE Solution under RTA

BTE solution for mobility defines relationship between scattering and mobility...

$$\Rightarrow \mu_n = \frac{< E\tau(E) >}{< E >} \frac{q}{m^*}$$

In the Boltzmann Limit...

$$< E > = \frac{3}{2} n k_B T_L$$

For Acoustic Deformation Potential Scattering...

$$\frac{1}{\tau(E)} = \frac{\pi D_A^2 k_B T_L}{\hbar \rho v_s^2} g(E)$$

$$< E\tau > = < \frac{1}{2} m^* v^2 \tau > = m^* \underbrace{< v^2 \tau >}$$

D = diffusion constant

$$\mu_n = \frac{q\, D}{k_B T_L}$$

Relaxation Time Approximation

$$\sum_{k'} \left(f(k')S(k',k) \,-\, f(k)S(k,k') \right)$$

$$= \sum_{k'} \left(f_S(k')S(k',k) \,-\, f_S(k)S(k,k') \right) + \sum_{k'} \left(f_A(k')S(k',k) \,-\, f_A(k)S(k,k') \right)$$

For low-field transport... $f_S(k) \approx f_o(k)$

$$\approx \sum_{k'} \left(f_A(k')S(k',k) \,-\, f_A(k)S(k,k') \right)$$

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

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

Relaxation Time Approximation

Detailed Balance

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

In equilibrium...

$$\sum_{k'} \left(f_o(k')S(k',k) \,-\, f_o(k)S(k,k') \right) = 0$$

Detailed Balance...

$$\frac{S(k',k)}{S(k,k')} = \frac{f_o(k)}{f_o(k')}$$

Out of equilibrium...

$$\frac{df}{dt} \approx -\sum_{k'} f_A(k)S(k,k') \left(1 - \frac{S(k',k)f_A(k')}{S(k,k')f_A(k)} \right) = -\sum_{k'} f_A(k)S(k,k') \left(1 - \frac{f_0(k)f_A(k')}{f_0(k')f_A(k)} \right)$$

Relaxation Time Approximation

Isotropic Scattering

$$\frac{df}{dt} = -f_A(k)\sum_{k'} S(k,k') + f_A(k)\left(\frac{f_o(k)}{f_A(k)}\right)\sum_{k'}\frac{S(k,k')f_A(k')}{f_o(k')}$$

$$S(k,k') = S(k,-k')$$

$$\Rightarrow \sum_{k'}\frac{S(k,k')f_A(k')}{f_0(k')} = 0$$

$$\Rightarrow \frac{df}{dt} = -f_A(k)\sum_{k'} S(k,k') = \frac{-f_A(k)}{\tau(k)}$$

Relaxation Time Approximation

Elastic Scattering

$$\frac{df}{dt} = -f_A(k)\sum_{k'} S(k,k') + f_A(k)\left(\frac{f_o(k)}{f_A(k)}\right)\sum_{k'}\frac{S(k,k')f_A(k')}{f_o(k')}$$

Low-field transport...

$$f_A(k) = \frac{-q\tau(K)f_o(k)\hbar}{k_B T_L m^*}\,\overline{E}\cdot\overline{k} = -a\tau(k)f_o(k)Ek\cos\theta$$

$$\frac{df}{dt} = -f_A(k)\sum_{k'} S(k,k')\left(1-\frac{f_o(k)\,a\,\tau(k')f_o(k')Ek'\cos\theta'}{f_o(k')\,a\,\tau(k)f_o(k)Ek\cos\theta}\right)$$

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

$$= -f_A(k)\sum_{k'} S(k,k')\left(1-\frac{\cos\theta'}{\cos\theta}\right)$$ (Elastic scattering $|k'| = |k|$)

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