6.730 Physics for Solid State Applications

Lecture 28: Scattering of Bloch Functions

Outline

- Review of Quasi-equilibrium
- Occupancy Functions
- Fermi's Golden Rule
- Bloch electron scattering

•Lundstrom, sec 1.7

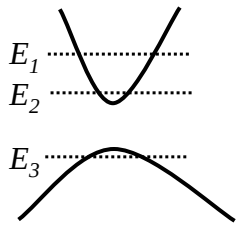
April 14, 2004

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...

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

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

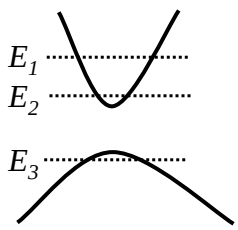
All the classical information about the carriers is contained in $f(r,k,t)$

Rate Equations for Occupancy Function

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

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

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



Now, generalize for the whole occupancy function...

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

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...

Fermi's Golden Rule from 2-state system

If a two state system with eigen energies E_1 and E_2, is driven by a sinusoidal potential such that the Hamiltonian is

$$H = \begin{pmatrix} E_1 & V_o e^{i\omega t} \\ V_o e^{-i\omega t} & E_2 \end{pmatrix}$$

Then if the system is initially in the 1-state, the probability of it going to the 2-state is, with $\omega_o = E_1 - E_2$

$$P(2) = \frac{(2V_o/\hbar)^2}{(\omega - \omega_o)^2 + (2V_o/\hbar)^2} \sin^2 \left\{ \sqrt{(\omega - \omega_o)^2 + (2V_o/\hbar)^2}\; t/2 \right\}$$

If the potential is small, then

$$P(2) = (2V_o/\hbar)^2 t^2 \left(\frac{\sin^2((\omega - \omega_o)t/2)}{(\omega - \omega_o)t/2} \right)^2$$

If the potential is small, then

$$P(2) = (2V_o/\hbar)^2 t^2 \left(\frac{\sin^2\left((\omega_2 - \omega_1 - \omega)t/2\right)}{(\omega_2 - \omega_1 - \omega)t/2} \right)^2$$

If there were many states to decay to, given by a density of states, g(ω), (not per unit volume), then the probability to decay to these states is

$$P = \int (2V_o/\hbar)^2 t^2 \underbrace{\left(\frac{\sin^2\left((\omega_j - \omega_1 - \omega)t/2\right)}{(\omega_j - \omega_1 - \omega)t/2} \right)^2}_{\lim_{t\to\infty} = 1 \quad \text{with width} \quad 2\pi/t} g(\omega_j)\, d\omega_j$$

$$\to \frac{2\pi}{t}\delta(\omega_j - \omega_1 - \omega)$$

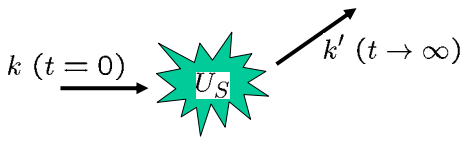
Therefore the rate, S = P/t is

$$S(1) = \int (2V_o/\hbar)^2\, \delta(\omega_j - \omega_1 - \omega)\, g(\omega_j)\, d\omega_j$$

$$= \sum_j S(1,j)$$

Fermi's Golden Rule

$S(k,k') =$ Scattering rate from *k* to *k'*



- For weak collisions to continuum of nearby states...

$$S(k,k') = \frac{|H_{k'k}|^2}{t\hbar^2}\left(t\,\frac{\sin(\frac{\Lambda t}{2})}{\frac{\Lambda t}{2}} \right)^2$$

where...

$$\hbar\Lambda = E(k') - E(k) - \hbar\omega$$

$$\lim_{T\to\infty} S(k,k') = \frac{|H_{k'k}|^2}{\hbar^2} 2\pi\,\hbar\delta(\Lambda) = \frac{|H_{k'k}|^2}{\hbar} 2\pi\,\delta(E(k') - E(k) - \hbar\omega)$$

- Energy conservation holds for infrequent collisions $t \to \infty$ ...

General Scattering Potential

We will only consider scattering potentials of the form...

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

$$= U^a(r,t) + U^e(r,t)$$

We can consider each potential term separately...

$$H^a_{k'k} = \int_V \psi_{nk'}(r)\ U^a_s(r,t)\ \psi_{nk}(r)\ d^3r$$

$$H^a_{k'k} = \int_V \psi_{nk'}(r)\ U^e_s(r,t)\ \psi_{nk}(r)\ d^3r$$

...Fermi...

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

General Scattering Potential

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

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

$U^a(r)\,e^{-i\omega t}$ final state energy is greater than initial → absorption

$U^e(r)\,e^{+i\omega t}$ final state energy is less than initial → emission

Matrix Elements for Bloch States

$$H_{k'k} = \int_V \psi_{nk'}(r)\, U_s(r,t)\, \psi_{nk}(r)\, d^3r$$

$$H_{k'k} = \int_{\frac{-L}{2}}^{\frac{L}{2}} \psi_{nk'}(z)\, U_s(z,t)\, \psi_{nk}(z)\, dz$$

$$= \int_{\frac{-L}{2}}^{\frac{L}{2}} u_{nk'}(z)\, \mathrm{e}^{-ik'z}\, U_s(z,t)\, u_{nk}(z)\, \mathrm{e}^{+ikz}\, dz$$

Approximation for slowly varying scattering potential…

$$\approx \sum_m \mathrm{e}^{-i(k'-k)z_m}\, U_s(z_m) \underbrace{\int_\Delta u_{nk'}(z) u_{nk}(z)\, dz}_{I(k,k';n,n')\ \text{Overlap integral}} \sim \frac{1}{N}$$

for n=n', and k=k'

Scattering from a Slowly Varying Potential

$$H_{k'k} \approx \sum_m \mathrm{e}^{-i(k'-k)z_m}\, U_s(z_m) \int_\Delta u_{nk'}(z) u_{nk}(z)\, dz$$

$$\approx \frac{1}{L} \int_{\frac{-L}{2}}^{\frac{L}{2}} U_s(z) \mathrm{e}^{-i(k'-k)z}\, dz$$

$$= U_s(k-k')$$

$$\int_\Delta u^*_{n,K}(r) u_{n,K}(r) d^3r = \frac{1}{N}$$

$$\frac{dz}{L} \approx \frac{\Delta}{L} = \frac{1}{N}$$

Matrix element is just the Fourier component $U_{s,k-k'}$ of the scattering potential at $q = k - k'$

For more quantitative work will need to evaluate overlap integral.

Scattering Rate Calculations

Example: 1-D Scattering from Defect

$$U_s(z) = A_o\delta(z) \qquad (1-D)$$

$$H_{k'k} = U_{s,k-k'} = \frac{1}{L}\int_{\frac{-L}{2}}^{\frac{L}{2}} A_o\delta(z)\ \mathrm{e}^{-i(k'-k)z}\,dz$$

$$= \frac{A_o}{L}$$

$\hbar\omega \to 0$ $\quad S(k,k') = \dfrac{2\pi}{\hbar}\ \dfrac{A_o^2}{L^2}\ \delta\left(E(k') - E(k)\right)$

- Sharply peaked potential scatters isotropically

$$indep.\ of\ \ q = k' - k$$

- Static potential scatters elastically

$$E(k') = E(k)$$

Scattering Rate Calculations

Example: 1-D Scattering from Traveling Wave

$$U_x(z,t) = A_\beta\ \mathrm{e}^{+i(\beta z - \omega t)}$$

$$H_{k'k} = \frac{1}{L}\int_{\frac{-L}{2}}^{\frac{L}{2}} A_\beta\ \mathrm{e}^{+i\beta z}\mathrm{e}^{-i(k'-k)z}\mathrm{e}^{-i\omega t}dz$$

$$= A_\beta\ \mathrm{e}^{-i\omega t}\,\delta_{k',k+\beta} \qquad \delta = 0 \text{ or } 1$$

$$S(k,k') = \frac{2\pi}{\hbar}\ |A_\beta|^2\ \delta\left(E(k') - E(k) - \hbar\omega\right)\delta_{k',k+\beta}$$

- Periodic potentials conserve total (crystal) momentum..

$$k' = k + \beta$$

Scattering Times

Scattering time out of state *k* ...

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

...at low densities...

$$\frac{1}{\tau(k)} \approx \sum_{k'} S(k,k')$$

...relaxation time is a function of state k

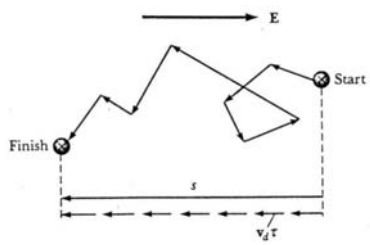
We usually measure some ensemble averaged relaxation time...$< \tau >$

...which means we have to know $f(r,k,t)$

Scattering Times

Relaxation time for z-directed momentum...

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



Relaxation time for energy...

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

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

$$< \tau >$$