6.730 Physics for Solid State Applications

Lecture 27: Scattering of Bloch Functions

Outline

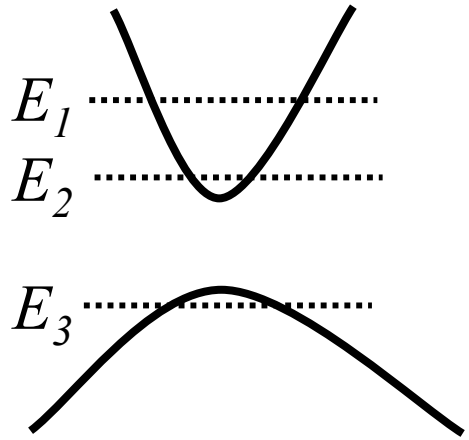
- Review of Quasi-equilibrium
- Occupancy Functions
- Fermi's Golden Rule
- Bloch electron scattering

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…

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

Quasi-equilibrium occupancy function…

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

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…

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

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

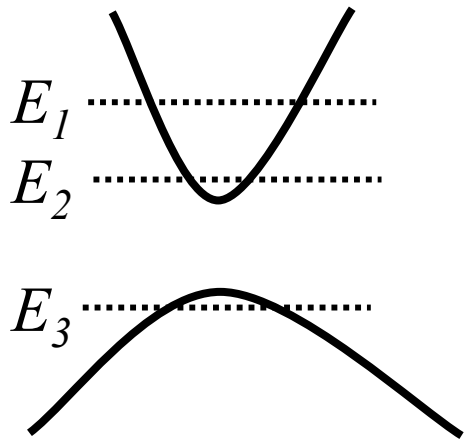
All the classical information about the carriers is contained in $f(r,k,t)$

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…

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

Rate Equations for Occupancy Function

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

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

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

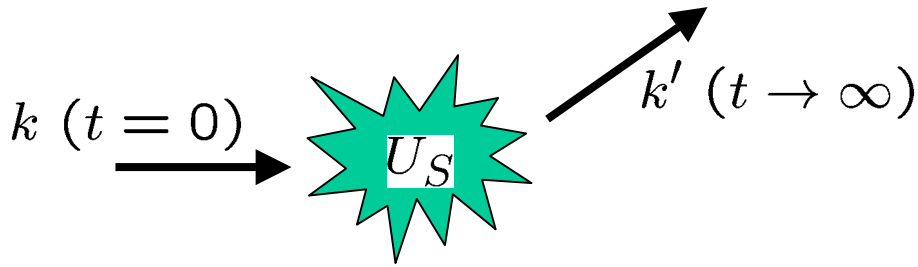
Perturbations that cause scattering….

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

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

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

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

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

Initial and Final States for Scattering

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

Envelope (effective mass) approximation…

$$\psi_{nk}(r) \approx G_n(r,t) u_{nk}(r)$$

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

Δ is volume of primitive cell

N is numer of primitive cells in solid

$\Rightarrow G_n(r,t)$ are slowly varying over Δ

$$\Rightarrow \left(-\frac{\hbar^2 \nabla^2}{2m^*} + E_c + V(r) \right) G_n(r,t) = i\hbar\, \partial_t G_n(r,t)$$

Normalization of Envelope Functions

$$1 = \int_V \psi_n^*(r,t)\psi_n(r,t)d^3r = \int_V G_n^*(r,t)G_n(r,t)u_{n,k}^*(r)u_{n,k}(r)d^3r$$

Since envelope functions are slowly varying…

$$1 \approx \sum_m G_n^*(R_m,t)G_n(R_m,t)\int_\Delta u_{nk}^*(r)u_{nk}(r)d^3r$$

$$= \frac{1}{N}\sum_m G_n^*(R_m,t)G_n(R_m,t)$$

$$= \frac{1}{V}\sum_m \Delta\ G_n^*(R_m,t)G_n(R_m,t)$$

$$= \frac{1}{V}\int_V G_n^*(R,t)G_n(R,t)d^3R$$

Normalization of envelope functions…

$$\int_V G_n^*(R,t)G_n(R,t)d^3R = V$$

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 periodic scattering potential…

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

Approximation for slowly varying scattering potential…

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

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 $q = k - k'$

Scattering Rate Calculations

Example: 1-D Scattering from Defect

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

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

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

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

- 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 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

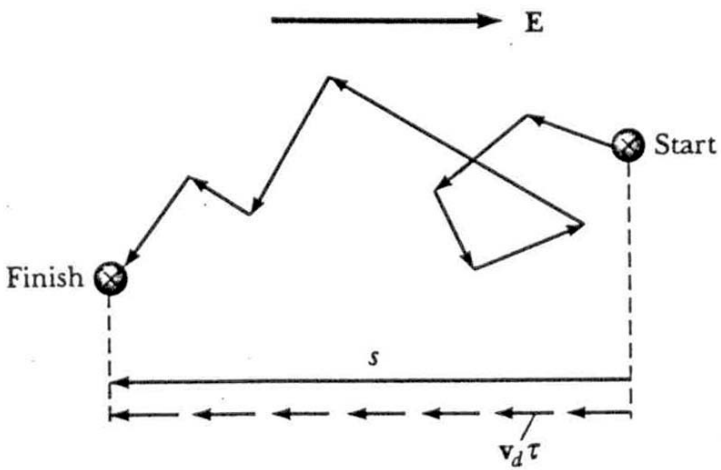
We usually measure some ensemble averaged relaxation time…$< \tau >$

…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…

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