Outline

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

\[ f(E) \quad \text{vs.} \quad f(k) \]
\[ f(E, r) \quad f(k, r) \]
\[ f(E, r, t) \quad f(k, r, t) \]

Equilibrium occupancy function...

\[ f_o(k, r) = \frac{1}{1 + e^{(E_{c}(r,k) - E_{F_0})/k_B T}} \]

Quasi-equilibrium occupancy function...

\[ f(k, r) \approx \frac{1}{1 + e^{(E_{c}(r,k) - E_{F_c}(r))/k_B T}} \]
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...

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

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

Now, generalize for the whole occupancy function...

\[
\frac{df(r, k, t)}{dt} = \sum_{k'} \left( \left( f(k') (1 - f(k)) S(k', k) - f(k) (1 - f(k')) S(k, k') \right) \right)
\]
Rate Equations for Occupancy Function

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\]

\[S(k', k)\] 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

\[ S(k, k') = \text{Scattering rate from } k \text{ to } k' \]

\[ k \ (t = 0) \rightarrow \underbrace{U_S}_{\text{interaction}} \rightarrow k' \ (t \rightarrow \infty) \]

- 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...

\[ \hbar \Lambda = E(k') - E(k) - \hbar \omega \]

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

- Energy conservation holds for infrequent collisions \( t \rightarrow \infty \) ...
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...

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

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

...Fermi...

\[ S(k, k') = \frac{2\pi}{\hbar} \left[ |H_{k'k}^a|^2 \delta(E(k') - E(k) - \hbar\omega) + |H_{k'k}^e|^2 \delta(E(k') - E(k) + \hbar\omega) \right] \]
General Scattering Potential

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

\[
S(k, k') = \frac{2\pi}{\hbar} \left[ |H_{k,k'}^{a}|^2 \delta(E(k') - E(k) - \hbar\omega) + |H_{k',k}^{e}|^2 \delta(E(k') - E(k) + \hbar\omega) \right]
\]

\[U^a(r) e^{-i\omega t} \quad \text{final state energy is greater than initial} \quad \rightarrow \quad \text{absorption}\]

\[U^e(r) e^{+i\omega t} \quad \text{final state energy is less than initial} \quad \rightarrow \quad \text{emission}\]
Initial and Final States for Scattering

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

Envelope (effective mass) approximation...

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

\[ \int_\Delta u_{n,k}^*(r) u_{n,k}(r) d^3r = \frac{1}{N} \]

\( \Delta \) is volume of primitive cell

\( N \) is number of primitive cells in solid

\[ G_n(r, t) \] are slowly varying over \( \Delta \)

\[ \left( -\frac{\hbar^2 \nabla^2}{2m^*} + E_c + V(r) \right) G_n(r, t) = i\hbar \partial_t G_n(r, t) \]
Normalization of Envelope Functions

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

Since envelope functions are slowly varying...

\[ 1 \approx \sum_m G_n^*(R_m, t) G_n(R_m, t) \int_\Delta u_{n,k}^*(r) u_{n,k}(r) d^3 r \]

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

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

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

Normalization of envelope functions...

\[ \int_V G_n^*(R, t) G_n(R, t) d^3 R = V \]
Matrix Elements for Bloch States

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

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

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

Approximation for periodic scattering potential...

\[ \approx \sum_m e^{-i(k'-k)zm} \int_{\Delta} u_{nk'}(z) U_s(z) u_{nk}(z) \, dz \]

Approximation for slowly varying scattering potential...

\[ \approx \sum_m e^{-i(k'-k)zm} U_s(z_m) \int_{\Delta} u_{nk'}(z) u_{nk}(z) \, dz \]
Scattering from a Slowly Varying Potential

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

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

\[ = U_{s,k-k'} \]

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

\[ \frac{dz}{L} \approx \frac{\Delta}{L} = \frac{1}{N} \]

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

\[ U_s(z) = A_o \delta(z) \quad (1 - D) \]

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

\[ = \frac{A_o}{L} \]

\[ \hbar \omega \rightarrow 0 \quad S(k, k') = \frac{2\pi}{\hbar} \frac{A_o^2}{L^2} \ \delta \left( E(k') - E(k) \right) \]

- Sharply peaked potential scatters isotropically
  \[ \text{indep. of } q = k' - k \]
- Static potential scatters elastically
  \[ E(k') = E(k) \]
Scattering Rate Calculations

Example: 1-D Scattering from Traveling Wave

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

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

\[ = A_\beta \ e^{-i\omega t} \delta(k' = k + \beta) \quad \delta = 0 \text{ or } 1 \]

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

- 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...

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