6.730 Physics for Solid State Applications

Lecture 28: Electron-phonon Scattering

Outline

- Bloch Electron Scattering
- Deformation Potential Scattering
- LCAO Estimation of Deformation Potential
- Matrix Element for Electron-Phonon Scattering
- Energy and Momentum Conservation

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

Scattering from a Slowly Varying Potential

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

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

$$= U_{s,k-k'}$$

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

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

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 Traveling Wave

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

$$H_{k'k} = \frac{1}{L} \int_{\frac{-L}{2}}^{\frac{L}{2}} A_\beta \; \mathrm{e}^{+i\beta z} \mathrm{e}^{-i(k'-k)z} dz$$

$$= A_\beta \;\; \delta(k' = k + \beta) \qquad\qquad \delta = 0 \text{ or } 1$$

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

- Periodic potentials conserve total momentum..

$$k' = k + \beta$$

Scattering 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

$$<\tau>$$

Electron-Phonon Scattering Potential

Beyond the Born-Oppenheimer Approximation…

- Phonons change the electron energies by changing the bond displacement
- Both shear strain and local volume changes alter the electron energy

…change in the bandstructure due to a dilatation of solid by sound wave…

$$H_{\text{e-ion}} = U_{\text{e-phonon}} \approx \frac{\partial H_{\text{e}}}{\partial V}\Big|_{eq.} \; \Delta V$$

$$\approx \frac{\partial E_n(k)}{\partial V}\Big|_{eq.} \Delta V = \left(\frac{\partial E_n(k)}{\partial V} \Big|_{eq.} V \right) \frac{\Delta V}{V}$$

$$D_A \equiv \; acoustic \; deformation \; potential \; = \left(\frac{\partial E_n(k)}{\partial V} \Big|_{eq.} V \right)$$

Relate the phonons to local changes in the volume (lattice constant)….

Electron-Phonon Scattering Potential

$$\text{e} = \frac{\Delta V}{V} = \sum_i E_{ii} = \sum_i \frac{\partial u_i}{\partial x_i} = \nabla \cdot \overline{u}$$

$$\overline{u}(r,t) = \overline{A}\ \sin(\overline{\beta} \cdot \overline{r} - \omega t)$$

$$\nabla \cdot \overline{u}(r,t) = \overline{\beta} \cdot \overline{u}(r,t)$$

$$\frac{\nabla V}{V} = \nabla \cdot \overline{u} = \overline{\beta} \cdot \overline{u}$$

$$\overline{\beta} \perp \overline{u} \qquad \frac{\nabla V}{V} \approx 0$$

$$\overline{\beta} \parallel \overline{u} \qquad \frac{\nabla V}{V} \neq 0$$

Only LA phonons cause local changes in the volume (lattice constant)….

Electron-Phonon Scattering Potential

$$U_{e-ph} = D_A \overline{\nabla} \cdot \overline{u}(r,t) = D_A \overline{\beta} \cdot \overline{u}(r,t)$$

$$D_A = \left(\frac{\partial E_n(k)}{\partial V} |_{eq.} V \right)$$

Conduction band (diamond):

$$E_c(\Gamma) = E_s + |4V_{ss\sigma}|$$

Valence band (diamond):

$$E_v(\Gamma) = E_p - |\frac{4}{3}V_{pp\sigma} - \frac{8}{3}V_{pp\pi}|$$

$$V_{ll'm} = \eta_{ll'm} \frac{\hbar^2}{md^2}$$

⇒

d ↓

$|V_{ll'm}|$ ↑

E_c ↑ ⇒ $D_{A_c} < 0$

E_v ↓ ⇒ $D_{A_v} > 0$

Electron-Phonon Scattering Potential

$$D_A = \frac{\partial E_n(k)}{\partial V}|_{eq}\ V$$

$$V_{ll'm} = \eta_{ll'm}\frac{\hbar^2}{md^2} \Rightarrow \frac{\partial V_{ll'm}}{\partial d}| = -2\,V_{ll'm}\,\frac{1}{d}$$

$$D_A = \frac{\partial E_n(\Gamma)}{\partial V}|_{eq} \cdot V = \frac{\partial E_n(\Gamma)}{\partial d}|_{eq} \cdot \frac{\partial d(\Gamma)}{\partial V}|_{eq} \cdot V = \frac{\partial E_n(\Gamma)}{\partial d}|_{eq} \cdot \frac{d}{3}$$

$$E_c(\Gamma) = E_s + |4V_{ss\sigma}| \Rightarrow D_{A_c} = -8|V_{ss\sigma}|\frac{1}{d} \cdot \frac{d}{3} = -\frac{8}{3}|V_{ss\sigma}|$$

$$E_v(\Gamma) = E_p - |\frac{4}{3}V_{pp\sigma} - \frac{8}{3}V_{pp\pi}| \Rightarrow D_{A_v} = +\frac{2}{3}\,|\frac{4}{3}V_{pp\sigma} - \frac{8}{3}V_{pp\pi}|$$

Electron-Phonon Scattering Potential

Silicon Example

$$D_A = \frac{\partial E_n(k)}{\partial V}|_{eq}\ V$$

$$D_{A_c} = -8|V_{ss\sigma}|\frac{1}{d}\cdot\frac{d}{3} = -\frac{8}{3}|V_{ss\sigma}|$$

$$= -5.42 \qquad \text{LCAO Theory}$$

$$D_{A_v} = +\frac{2}{3}\ |\frac{4}{3}V_{pp\sigma} - \frac{8}{3}V_{pp\pi}|$$

$$= +1.75 \qquad \text{LCAO Theory}$$

$$a_c - a_v = D_{A_c} - D_{A_v}$$

$$= -7.17 \qquad \text{LCAO Theory}$$

$$= -10 \qquad \text{Approx Experiment}$$

Phonon Displacement Operator

$$U_{e-ph} = D_A \nabla \cdot \overline{U}(r,t) = D_A \, \overline{\beta} \cdot \overline{U}_\beta(r,t)$$

See Lecture 11…phonon displacement operator

$$\hat{U}_\beta(r,t) = \sum_\beta \sqrt{\frac{\hbar}{2\rho V \omega_\beta}} \left(\hat{a}_\beta e^{i(\beta r - \omega t)} + \hat{a}_\beta^\dagger e^{-i(\beta r - \omega t)} \right) \overline{\epsilon}_\beta$$

relating mass for continuum solid and discrete lattice $\rho V \equiv MN$

$$U_{e-ph} = \sum_\beta D_A \, (\overline{\beta} \cdot \overline{\epsilon}_\beta) \sqrt{\frac{\hbar}{2\rho V \omega_\beta}} \left(\hat{a}_\beta e^{i(\beta r - \omega t)} + \hat{a}_\beta^\dagger e^{-i(\beta r - \omega t)} \right)$$

Scattering Rate Calculations

Overview

Step 1: Determine Scattering Potential

$$U_{e-ph} = \sum_{\beta} D_A \left(\overline{\beta} \cdot \overline{\epsilon}_{\beta}\right) \sqrt{\frac{\hbar}{2\rho V \omega_{\beta}}} \left(\hat{a}_{\beta} e^{i(\beta r - \omega t)} + \hat{a}_{\beta}^{\dagger} e^{-i(\beta r - \omega t)}\right)$$

Step 2: Calculate Matrix Elements

Step 3: Calculate State-State Transition Rates

Step 4: Calculate State Lifetime

Step 5: Calculate Ensemble Lifetime

Electron-Phonon Matrix Element

$$U_{e-ph} = \sum_{\beta} D_A \, (\overline{\beta}\cdot\overline{\epsilon}_\beta) \sqrt{\frac{\hbar}{2\rho V \omega_\beta}} \left(\hat{a}_\beta e^{i(\beta r - \omega t)} + \hat{a}_\beta^\dagger e^{-i(\beta r - \omega t)}\right)$$

Phonon absorption…

$$|\psi_i> = |\psi_{nk}> |n_\beta> = |\psi_{nk}, n_\beta>$$

$$|\psi_f> = |\psi_{nk'}> |n_\beta - 1> = |\psi_{nk}, n_\beta - 1>$$

$$H_{kk'} = \sum_{\beta} \sqrt{\frac{\hbar}{2\rho V \omega_\beta}} \left(\overline{\beta}\cdot\overline{\epsilon}_\beta\right) D_A \left\langle \psi_{nk'}, n_\beta - 1 \left| \hat{a}_\beta e^{+i\beta r} \right| \psi_{nk}, n_\beta \right\rangle$$

$$+ \sum_{\beta} \sqrt{\frac{\hbar}{2\rho V \omega_\beta}} \left(\overline{\beta}\cdot\overline{\epsilon}_\beta\right) D_A \left\langle \psi_{nk'}, n_\beta + 1 \left| \hat{a}_\beta^\dagger e^{-i\beta r} \right| \psi_{nk}, n_\beta \right\rangle$$

Electron-Phonon Matrix Element

$$H_{kk'} = \sum_{\beta} \sqrt{\frac{\hbar}{2\rho V \omega_\beta}} \left(\overline{\beta} \cdot \overline{\epsilon}_\beta\right) D_A \left\langle \psi_{nk'}, n_\beta - 1 \left| \hat{a}_\beta e^{+i\beta r} \right| \psi_{nk}, n_\beta \right\rangle$$

$$+ \sum_{\beta} \sqrt{\frac{\hbar}{2\rho V \omega_\beta}} \left(\overline{\beta} \cdot \overline{\epsilon}_\beta\right) D_A \left\langle \psi_{nk'}, n_\beta + 1 \left| \hat{a}^\dagger_\beta e^{-i\beta r} \right| \psi_{nk}, n_\beta \right\rangle$$

$$H_{KK'} = \sum_{\beta} \sqrt{\frac{\hbar}{2\rho V \omega_\beta}} \left(\overline{\beta} \cdot \overline{\epsilon}_\beta\right) D_A \left(\left\langle \psi_{nk'} \left| e^{i\beta \cdot r} \right| \psi_{nk} \right\rangle \sqrt{n_\beta} + \left\langle \psi_{nk'} \left| e^{-i\beta \cdot r} \right| \psi_{nk} \right\rangle \sqrt{n_\beta + 1} \right)$$

For long wavelength phonons, can make slowly-varying approx… $\beta \ll \frac{\pi}{a}$

$$= \sum_{\beta} \sqrt{\frac{\hbar}{2\rho V \omega_\beta}} \left(\overline{\beta} \cdot \overline{\epsilon}_\beta\right) D_A \left(\sqrt{n_\beta}\ \delta_{k'=k+\beta} + \sqrt{n_\beta + 1}\ \delta_{k'=k-\beta} \right)$$

Scattering Rate Calculations

Overview

Step 1: Determine Scattering Potential

$$U_{e-ph} = \sum_{\beta} D_A \, (\overline{\beta} \cdot \overline{\epsilon}_\beta) \sqrt{\frac{\hbar}{2\rho V \omega_\beta}} \left(\hat{a}_\beta e^{i(\beta r - \omega t)} + \hat{a}_\beta^\dagger e^{-i(\beta r - \omega t)} \right)$$

Step 2: Calculate Matrix Elements

$$H_{kk'} = \sum_{\beta} \sqrt{\frac{\hbar}{2\rho V \omega_\beta}} \left(\overline{\beta} \cdot \overline{\epsilon}_\beta\right) D_A \left(\sqrt{n_\beta} \;\; \delta_{k'=k+\beta} + \sqrt{n_\beta + 1} \;\; \delta_{k'=k-\beta} \right)$$

Step 3: Calculate State-State Transition Rates

Step 4: Calculate State Lifetime

Step 5: Calculate Ensemble Lifetime

Electron-Phonon Scattering Rate

$$\left|H^a_{kk'}\right|^2 = \frac{\hbar}{2\rho V \omega_\beta}\,\beta^2 D_A^2\; n_\beta\;\; \delta_{k'=k+\beta}$$

$$\left|H^a_{kk'}\right|^2 = \frac{\hbar}{2\rho V \omega_\beta}\,\beta^2 D_A^2\; (n_\beta + 1)\;\; \delta_{k'=k-\beta}$$

$$S(k,k') = \frac{\pi}{\rho V \omega_\beta}\beta^2 D_A^2\; n_\beta\;\; \delta_{k'=k+\beta}\;\; \delta\left(E(k') - E(k) - \hbar\omega_\beta\right)$$

$$+ \frac{\pi}{\rho V \omega_\beta}\beta^2 D_A^2\; (n_\beta + 1)\;\; \delta_{k'=k-\beta}\;\; \delta\left(E(k') - E(k) + \hbar\omega_\beta\right)$$

Scattering Rate Calculations

Overview

Step 1: Determine Scattering Potential

$$U_{e-ph} = \sum_{\beta} D_A \left(\overline{\beta} \cdot \overline{\epsilon}_{\beta}\right) \sqrt{\frac{\hbar}{2\rho V \omega_{\beta}}} \left(\hat{a}_{\beta} e^{i(\beta r - \omega t)} + \hat{a}_{\beta}^{\dagger} e^{-i(\beta r - \omega t)}\right)$$

Step 2: Calculate Matrix Elements

$$H_{kk'} = \sum_{\beta} \sqrt{\frac{\hbar}{2\rho V \omega_{\beta}}} \left(\overline{\beta} \cdot \overline{\epsilon}_{\beta}\right) D_A \left(\sqrt{n_{\beta}}\ \delta_{k'=k+\beta} + \sqrt{n_{\beta}+1}\ \delta_{k'=k-\beta}\right)$$

Step 3: Calculate State-State Transition Rates

$$S(k,k') = \frac{\pi}{\rho V \omega_{\beta}} \beta^2 D_A^2\ n_{\beta}\ \delta_{k'=k+\beta}\ \delta\left(E(k') - E(k) - \hbar\omega_{\beta}\right)$$
$$+ \frac{\pi}{\rho V \omega_{\beta}} \beta^2 D_A^2\ (n_{\beta}+1)\ \delta_{k'=k-\beta}\ \delta\left(E(k') - E(k) + \hbar\omega_{\beta}\right)$$

Step 4: Calculate State Lifetime

Step 5: Calculate Ensemble Lifetime

Energy and Momentum Conservation

$$\hbar\overline{k'} = \hbar\overline{k} \pm \hbar\overline{\beta}$$

$$E(k') = E(k) \pm \hbar\omega_\beta$$

$$\frac{\hbar^2 k'^2}{2m^*} = \frac{\hbar^2 k^2}{2m^*} \pm \hbar\omega_\beta$$

$$\overline{k}'\cdot\overline{k}' = \overline{k}\cdot\overline{k} \pm 2\overline{k}\cdot\overline{\beta} + \overline{\beta}\cdot\overline{\beta} = k^2 + \beta^2 \pm 2k\beta\cos\theta$$

$$\frac{\hbar^2 k^2}{2m^*} + \frac{\hbar^2 \beta^2}{2m^*} \pm \frac{2\hbar^2 k\beta\cos\theta}{2m^*} = \frac{\hbar^2 k^2}{2m^*} \pm \hbar\omega_\beta$$

Energy and Momentum Conservation

$$\hbar \overline{k'} = \hbar \overline{k} \pm \hbar \overline{\beta} \qquad E(k') = E(k) \pm \hbar\omega_\beta$$

$$\boxed{\cancel{\frac{\hbar^2 k^2}{2m^*}} + \frac{\hbar^2 \beta^2}{2m^*} \pm \frac{2\hbar^2 k\beta \cos\theta}{2m^*} = \cancel{\frac{\hbar^2 k^2}{2m^*}} \pm \hbar\omega_\beta} \times \frac{2m^*}{\hbar\beta}$$

$$\hbar\beta = \mp 2\hbar k \cos\theta \pm \frac{2m^*}{\hbar\beta} \cdot \hbar\omega_\beta$$

For acoustic phonons… $\beta \ll \frac{\pi}{a}$

$$\omega_\beta = v_s\beta \;\Rightarrow\; \hbar\beta = \mp 2\hbar k \cos\theta \pm 2m^* v_s$$

$$= 2\hbar k \left(\mp \cos\theta \pm \frac{m^* v_s}{\hbar k} \right)$$

Energy and Momentum Conservation

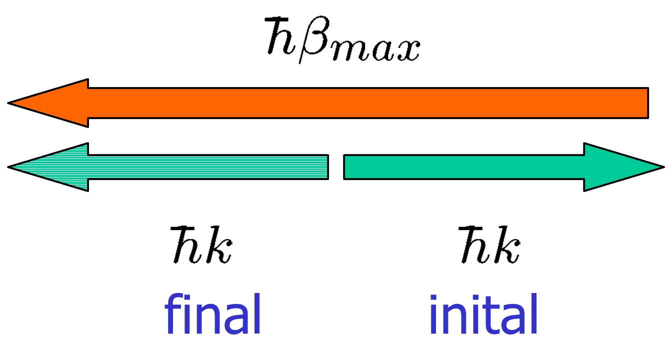
$$\hbar\beta = 2\hbar k\left(\mp\cos\theta \pm \frac{m^* v_s}{\hbar k}\right)$$

Typical acoustic phonon velocity… $v_s \approx 10^4 cm/s$

Velocity of typical electron (300 K)… $v_{th} \approx 10^7 cm/s$

$$\hbar\beta \approx 2\hbar k(\mp\cos\theta)$$

$$\hbar\beta_{max} = 2\hbar k$$



Energy and Momentum Conservation

Maximum momentum exchange…

$$\hbar\beta_{max} = 2\hbar k$$

Maximum energy exchange…

$$\hbar\omega_{\beta_{max}} = \hbar\beta_{max}v_s \approx 2\cdot(m^* v_{th})v_s$$

$$\approx 2\left(\frac{1}{20}\cdot 10^{-30}[kg]\cdot 10^{7}[cm/s]\right)10^{5}[cm/s]$$

$$\approx 2\left(\frac{1}{20}\cdot 10^{-30}[kg]\cdot 10^{5}[m/s]\right)10^{3}[m/s]$$

$$\approx 10^{-4}[eV] = 0.1[meV]$$

Acoustic phonon scattering is essentially elastic for 300K electrons…

Scattering Rate Calculations

Overview

Step 1: Determine Scattering Potential

$$U_{e-ph} = \sum_{\beta} D_A \; (\overline{\beta} \cdot \overline{\epsilon}_{\beta}) \sqrt{\frac{\hbar}{2\rho V \omega_{\beta}}} \; \left(\hat{a}_{\beta} e^{i(\beta r - \omega t)} + \hat{a}_{\beta}^{\dagger} e^{-i(\beta r - \omega t)} \right)$$

Step 2: Calculate Matrix Elements

$$H_{kk'} = \sum_{\beta} \sqrt{\frac{\hbar}{2\rho V \omega_{\beta}}} \left(\overline{\beta} \cdot \overline{\epsilon}_{\beta} \right) D_A \left(\sqrt{n_{\beta}} \;\; \delta_{k'=k+\beta} + \sqrt{n_{\beta}+1} \;\; \delta_{k'=k-\beta} \right)$$

Step 3: Calculate State-State Transition Rates

$$S(k,k') = \frac{\pi}{\rho V \omega_{\beta}} \beta^2 D_A^2 \; n_{\beta} \;\; \delta_{k'=k+\beta} \;\; \delta\left(E(k') - E(k) - \hbar\omega_{\beta} \right)$$
$$+ \frac{\pi}{\rho V \omega_{\beta}} \beta^2 D_A^2 \; (n_{\beta}+1) \;\; \delta_{k'=k-\beta} \;\; \delta\left(E(k') - E(k) + \hbar\omega_{\beta} \right)$$

Step 4: Calculate State Lifetime

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

Step 5: Calculate Ensemble Lifetime

Energy and Momentum Conservation

$$E(k') = E(k) \pm \hbar\omega_\beta$$

$$\frac{\hbar^2 k^2}{2m^*} + \frac{\hbar^2 \beta^2}{2m^*} \pm \frac{2\hbar^2 k\beta \cos\theta}{2m^*} = \frac{\hbar^2 k^2}{2m^*} \pm \hbar\omega_\beta$$

$$\delta\left(E(k') - E(k) \mp \hbar\omega_\beta\right) = \delta\left(\frac{\hbar^2 k\beta}{m^*}\left(\pm\cos\theta + \frac{\beta}{2k} \mp \frac{m^* v_s}{\hbar k}\right)\right)$$

$$= \frac{m^*}{\hbar^2 k\beta}\,\delta\left(\pm\cos\theta + \frac{\beta}{2k} \mp \frac{m^* v_s}{\hbar k}\right)$$

Electron-Phonon Scattering Time

Preview

$$S(k,k') = \frac{\pi}{\rho V \omega_\beta}\ \beta^2 D_A^2\ n_\beta\ \left(\frac{m^*}{\hbar^2 k \beta}\right) \delta\left(+\cos\theta + \frac{\beta}{2K} - \frac{m^* v_s}{\hbar k}\right)$$

$$+ \frac{\pi}{V \omega_\beta}\ \beta^2 D_A^2\ (n_\beta + 1)\ \left(\frac{m^*}{\hbar^2 k \beta}\right) \delta\left(-\cos\theta + \frac{\beta}{2k} + \frac{m^* v_s}{\hbar k}\right)$$

$$\frac{1}{\tau(k)} = \sum_{k'} S(k,k') = \sum_{\beta} S(k,k') = \frac{V}{8\pi^3} \int_0^{2\pi} d\phi \int_0^{\infty} \int_{-1}^{1} S(k,k') d\beta\ d(\cos\theta)$$