6.730 Physics for Solid State Applications

Lecture 30: Electron-phonon Scattering II

Outline

- Review of Last Time
- State-state Scattering Rate
- Electron-phonon Scattering Time
- Example: Silicon

April 23, 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

$$<\tau>$$

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

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

Step 5: Calculate Ensemble Lifetime $\langle \tau \rangle$

Energy and Momentum Conservation

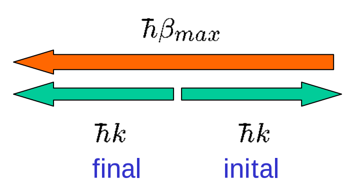
$$\hbar\beta = 2\hbar k \left(\mp \cos\theta \pm \frac{m^* v_s}{\hbar k}\right)$$

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...

Phonon Occupancy

Phonon number is given by Bose-Einstein distributon...

$$\Rightarrow n_\beta = \frac{1}{e^{\hbar\omega_\beta/k_B T_L} - 1}$$

$$\hbar\omega_{\beta_{max}} \approx 10^{-4}eV \qquad\qquad k_B T_L \approx 26meV$$

The minimum phonon number for any mode interacting with the electrons is...

$$n_\beta \approx \frac{1}{1+\frac{\hbar\omega_\beta}{k_B T_L}-1} \approx \frac{k_B T_L}{\hbar\omega_\beta} \sim 260 = \frac{k_B T_L}{\hbar v_s \beta}$$

$$n_\beta + 1 \approx n_\beta$$

Since the phonon number is large, spontaneous emission is negligible

Energy and Momentum Conservation

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

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

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

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

Energy and Momentum Conservation

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

...can collapse the energy & momentum conservation into a single δ-function

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

Electron-Phonon Scattering Time

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

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

Since phonon number is large... $n_\beta + 1 \approx n_\beta$

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

$$S(k,k') = \frac{\pi D_A^2 k_B T_L m^*}{\rho V v_s \hbar^3 v_s k}\ \beta^{-1}\left[\delta\left(\cos\theta + \frac{\beta}{2k} - \frac{m^* v_s}{\hbar k}\right) + \delta\left(-\cos\theta + \frac{\beta}{2k} + \frac{m^* v_s}{\hbar k}\right)\right]$$

Electron-Phonon Scattering Time

Can convert the sum over final states to a sum over phonons...

$$\hbar\bar{k'} = \hbar\bar{k} \pm \hbar\bar{\beta} \quad \Rightarrow \quad \frac{1}{\tau(k)} = \sum_{k'} S(k,k') = \sum_{\beta} S(k,k')$$

$$\frac{1}{\tau(k)} = \sum_{\beta} S(k,k') = \int S(k,k')\frac{d^3\beta}{(\frac{2\pi}{L})^3}$$

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

$$S(k,k') = \frac{\pi D_A^2 k_B T_L m^*}{\rho V v_s \hbar^3 v_s k}\ \beta^{-1}\Bigg[\delta\underbrace{\left(\cos\theta + \frac{\beta}{2k} - \frac{m^* v_s}{\hbar k}\right)}_{\text{absorption}} + \delta\underbrace{\left(-\cos\theta + \frac{\beta}{2k} + \frac{m^* v_s}{\hbar k}\right)}_{\text{emission}}\Bigg]$$

Electron-Phonon Absorption Time

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

$$= \frac{V}{8\pi^3}\int_0^{2\pi} d\phi \int_0^{\infty} \beta \int_{-1}^{1} \delta\left(\cos\theta + \frac{\beta}{2k} - \frac{m^* v_s}{\hbar k}\right) d(\cos\theta) * \left(\frac{\pi D_A^2 k_B T_L m^*}{\rho V v_s \hbar^3 k}\right)$$

$$= \frac{D_A^2 k_B T_L m^*}{4\pi\rho v_s^2 \hbar^3 k}\int_0^{\infty} \beta \int_{-1}^{1} \delta\left(\cos\theta + \frac{\beta}{2k} - \frac{m^* v_s}{\hbar k}\right) d(\cos\theta)$$

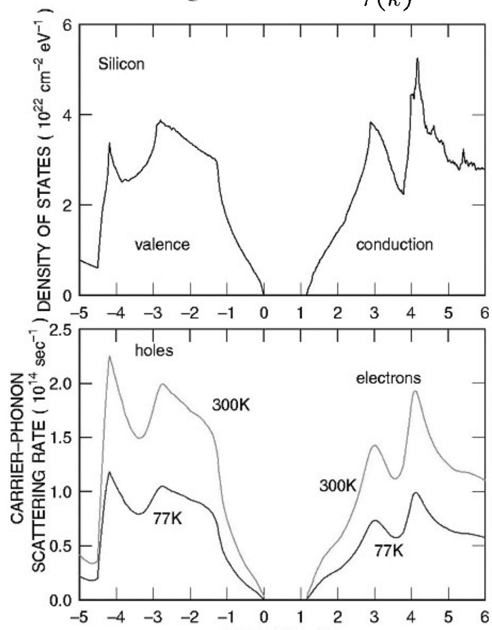
$$= \frac{D_A^2 k_B T_L m^*}{4\pi\rho v_s^2 \hbar^3 k}\int_0^{\beta_{max}} \beta \, d\beta = \frac{D_A^2 k_B T_L m^*}{4\pi\rho v_s^2 \hbar^3 k}\frac{\beta_{max}^2}{2}$$

$$= \frac{D_A^2 k_B T_L m^*}{4\pi\rho v_s^2 \hbar^3 k}\frac{4\hbar^2 k^2}{2} = \frac{D_A^2 k_B T_L m^* k}{2\pi\rho v_s^2 \hbar^3}$$

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

Electron-Phonon Scattering Rate

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



Electron-Phonon Scattering Time

Silicon Example

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

Density-of-states

- ½ conventional value since electron-phonon scattering doesn't flip spin
- Need to account for ellipsoidal valleys in Si conduction band
- Need to account for 6 equivalent valleys

$$g_c(E) = \frac{1}{2\pi^2}\left(\frac{2m_d^*}{\hbar^2}\right)^{3/2}\sqrt{E}$$

$$m_d^{*3/2} = 6(m_x^* m_y^* m_z^*)^{1/2} = 6(m_l^* m_t^{*2})^{1/2}$$

$m_l^* = 0.916 m_o$ $\quad$ $m_t^* = 0.19 m_o$ $\quad$ → $\quad$ $m_d^* = 1.06 m_o$

Electron-Phonon Scattering Time

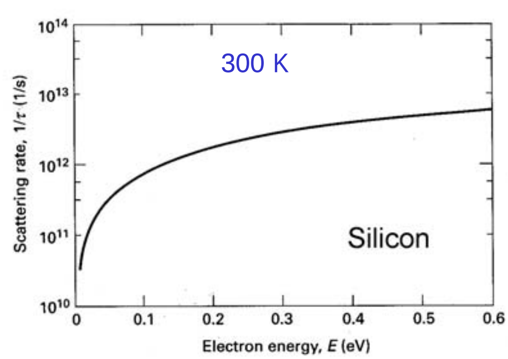
Silicon Example

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

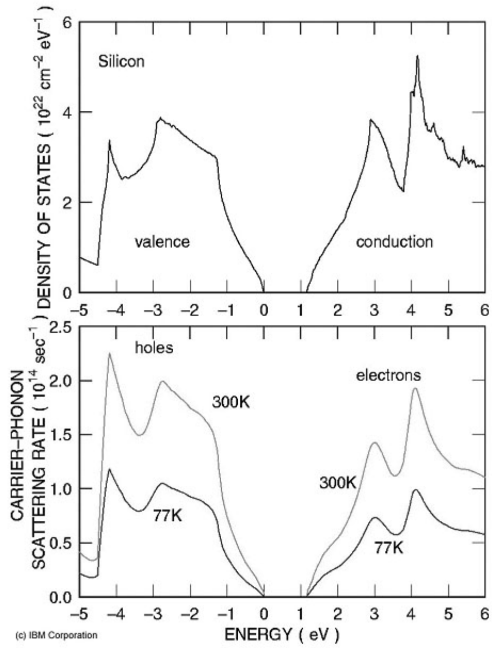
$D_A = 9.5\,\mathrm{eV}$

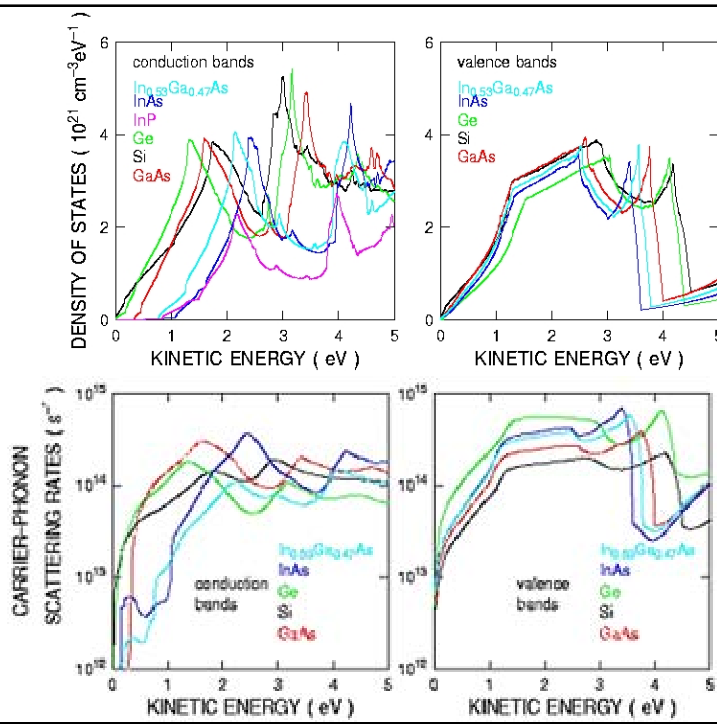
$v_s = 9.04\text{x}10^5\,\mathrm{cm/s}$

$\rho = 3.29\,\mathrm{g/cm^3}$



Electron-Phonon Scattering Rate





Scattering Rate Calculations

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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

$$S(k,k') = \frac{\pi}{\rho V \omega_{\beta}} \beta^2 D_A^2 \, n_{\beta} \; \delta_{k'=k+\beta} \; \delta\left(E(k') - E(k) - \hbar\omega_{\beta} \right)$$
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Step 4: Calculate State Lifetime

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

Step 5: Calculate Ensemble Lifetime

$$< \tau >$$