

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 slowly varying scattering potential...

$$\approx \sum_{m} e^{-i(k'-k)z_{m}} U_{s}(z_{m}) \int_{\Delta} u_{nk'}(z)u_{nk}(z) dz$$

$$I(k, k'; n, n') \text{ Overlap integral} \sim \frac{1}{N}$$
for n=n', and k=k'

Scattering from a Slowly Varying Potential

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

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

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

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

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

2

Scattering Rate Calculations
Example: 1-D Scattering from Traveling Wave

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

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

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

$$S(k,k') = \frac{2\pi}{\hbar} |A_\beta|^2 \ \delta \left(E(k') - E(k) - \hbar\omega \right) \delta(k' = k + \beta)$$
• Periodic potentials conserve total momentum.

$$k' = k + \beta$$

Scattering 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

$$H^{a}_{k'k} = \int_{V} \psi_{nk'}(r) \ U^{a}_{s}(r) \ \psi_{nk}(r) \ d^{3}r$$

Step 3: Calculate State-State Transition Rates

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

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...

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

$$pprox rac{\partial E_n(k)}{\partial V}|_{eq.}\Delta V = \left(rac{\partial E_n(k)}{\partial V} \;|_{eq.}V
ight)rac{\Delta V}{V}$$

$$D_A \equiv a constic \ deformation \ potential \ = \left(rac{\partial E_n(k)}{\partial V} \mid_{eq.} V
ight)$$

Relate the phonons to local changes in the volume (lattice constant).... Lundstom, 2.2.2

Electron-Phonon Scattering Potential

$$e = \frac{\Delta V}{V} = \sum_{i} E_{ii} = \sum_{i} \frac{\partial u_{i}}{\partial x_{i}} = \nabla \cdot \overline{u}$$

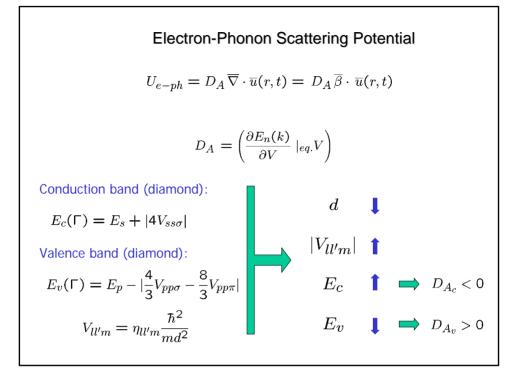
$$\overline{u}(r,t) = \overline{A} \sin(\overline{\beta} \cdot \overline{r} - \omega t)$$

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

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

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

$$\overline{\beta} \parallel \overline{u} \qquad \frac{\nabla V}{V} \neq 0$$
Only LA phonons cause local changes in the volume (lattice constant)....



Electron-Phonon Scattering Potential

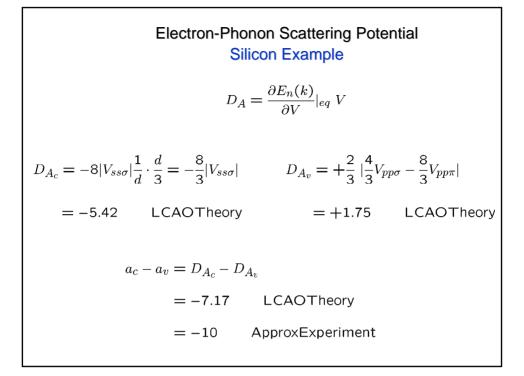
$$D_{A} = \frac{\partial E_{n}(k)}{\partial V}|_{eq} V$$

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

$$D_{A} = \frac{\partial E_{n}(\Gamma)}{\partial V}|_{eq} V = \frac{\partial E_{n}(\Gamma)}{\partial d}|_{eq} \cdot \frac{\partial d(\Gamma)}{\partial V}|_{eq} \cdot V = \frac{\partial E_{n}(\Gamma)}{\partial d}|_{eq} \cdot \frac{d}{3}$$

$$E_{c}(\Gamma) = E_{s} + |4V_{ss\sigma}| \longrightarrow D_{A_{c}} = -8|V_{ss\sigma}|\frac{1}{d} \cdot \frac{d}{3} = -\frac{8}{3}|V_{ss\sigma}|$$

$$E_{v}(\Gamma) = E_{p} - |\frac{4}{3}V_{pp\sigma} - \frac{8}{3}V_{pp\pi}| \longrightarrow D_{A_{v}} = +\frac{2}{3}|\frac{4}{3}V_{pp\sigma} - \frac{8}{3}V_{pp\pi}|$$



From Lecture 12:

$$\begin{aligned} H &= \sum_{\mathbf{k}} \sum_{\sigma} \hbar \omega_{\mathbf{k}\sigma} \left[a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma} + \frac{1}{2} \right] \\ \hat{a}_{\mathbf{k}\sigma} &= \sum_{\mathbf{R}_{j}} \frac{e^{-i\mathbf{k}\mathbf{R}_{j}}}{\sqrt{N}} \vec{\epsilon}_{\mathbf{k}\sigma} \left(\sqrt{\frac{M\omega_{\mathbf{k}\sigma}}{2\hbar}} \mathbf{u}[\mathbf{R}_{j}, \mathbf{t}] + i\sqrt{\frac{1}{2M\hbar\omega_{\mathbf{k}\sigma}}} \mathbf{M}\dot{\mathbf{u}}[\mathbf{R}_{j}, \mathbf{t}] \right) \\ \hat{a}_{\mathbf{k}\sigma}^{\dagger} &= \sum_{\mathbf{R}_{j}} \frac{e^{i\mathbf{k}\mathbf{R}_{j}}}{\sqrt{N}} \vec{\epsilon}_{\mathbf{k}\sigma} \left(\sqrt{\frac{M\omega_{\mathbf{k}\sigma}}{2\hbar}} \mathbf{u}[\mathbf{R}_{j}, \mathbf{t}] - i\sqrt{\frac{1}{2M\hbar\omega_{\mathbf{k}\sigma}}} \mathbf{M}\dot{\mathbf{u}}[\mathbf{R}_{j}, \mathbf{t}] \right) \\ \mathbf{u}[\mathbf{R}_{j}, \mathbf{t}] &= \sum_{\mathbf{k}\sigma} \sqrt{\frac{\hbar}{2MN\omega_{\mathbf{k}\sigma}}} \left(\hat{a}_{\mathbf{k}\sigma} e^{i\mathbf{k}\mathbf{R}_{j}} + \hat{a}_{\mathbf{k}^{\dagger}\sigma} e^{-i\mathbf{k}\mathbf{R}_{j}} \right) \tilde{\epsilon}_{\mathbf{k}\sigma} \end{aligned}$$

We will now use this for electron-phonon scattering...

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 12...phonon displacement operator, with time dependence, $\mathbf{u}[\mathbf{R}_{\mathbf{j}}, \mathbf{t}] = \sum_{\mathbf{k}\sigma} \sqrt{\frac{\overline{h}}{2MN\omega_{\mathbf{k}\sigma}}} \left(\hat{\mathbf{a}}_{\mathbf{k}\sigma} \mathbf{e}^{\mathbf{i}\mathbf{k}\mathbf{R}_{\mathbf{j}}} + \hat{\mathbf{a}}_{\mathbf{k}^{\dagger}\sigma} \mathbf{e}^{-\mathbf{i}\mathbf{k}\mathbf{R}_{\mathbf{j}}} \right) \tilde{\epsilon}_{\mathbf{k}\sigma}$ $\implies \widehat{U}_{\beta}(r,t) = \sum_{\beta} \sqrt{\frac{\overline{h}}{2\rho V \omega_{\beta}}} \left(\hat{a}_{\beta} e^{i(\beta r - \omega t)} + \hat{a}_{\beta}^{\dagger} e^{-i(\beta r - \omega t)} \right) \bar{\epsilon}_{\beta}$ relating mass for continuum solid and discrete lattice $\rho V \equiv MN$ $U_{e-ph} = \sum_{\beta} D_A \left(\overline{\beta} \cdot \overline{\epsilon}_{\beta} \right) \sqrt{\frac{\overline{h}}{2\rho V \omega_{\beta}}} \left(\hat{a}_{\beta} e^{i(\beta r - \omega t)} + \hat{a}_{\beta}^{\dagger} e^{-i(\beta r - \omega t)} \right)$

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

$$\begin{split} \text{Electron-Phonon Matrix Element} \\ U_{e-ph} &= \sum_{\beta} D_A \left(\overline{\beta} \cdot \overline{\epsilon}_{\beta} \right) \sqrt{\frac{\overline{h}}{2\rho V \omega_{\beta}}} \left(\hat{a}_{\beta} e^{i(\beta r - \omega t)} + \hat{a}_{\beta}^{\dagger} e^{-i(\beta r - \omega t)} \right) \\ \text{Consider the coupled electron-phonon wavefunction} \\ &|\psi_i \rangle &= |\psi_{nk} \rangle |n_{\beta} \rangle &= |\psi_{nk}, n_{\beta} \rangle \\ \text{Phonon absorption} \dots \quad |\psi_f \rangle &= |\psi_{nk'} \rangle |n_{\beta} - 1 \rangle &= |\psi_{nk'}, n_{\beta} - 1 \rangle \\ \text{Phonon emission} \dots \quad |\psi_f \rangle &= |\psi_{nk'} \rangle |n_{\beta} + 1 \rangle &= |\psi_{nk'}, n_{\beta} + 1 \rangle \\ H_{kk'} &= \sum_{\beta} \sqrt{\frac{\overline{h}}{2\rho V \omega_{\beta}}} \left(\overline{\beta} \cdot \overline{\epsilon}_{\beta} \right) D_A \left\langle \psi_{nk'}, n_{\beta} - 1 \right| \hat{a}_{\beta} e^{-i\beta r} |\psi_{nk}, n_{\beta} \right\rangle \\ &+ \sum_{\beta} \sqrt{\frac{\overline{h}}{2\rho V \omega_{\beta}}} \left(\overline{\beta} \cdot \overline{\epsilon}_{\beta} \right) D_A \left\langle \psi_{nk'}, n_{\beta} + 1 \right| \hat{a}_{\beta}^{\dagger} e^{-i\beta r} |\psi_{nk}, n_{\beta} \rangle \end{split}$$

Electron-Phonon Matrix Element

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

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

$$H_{kk'} = \sum_{\beta} \sqrt{\frac{\hbar}{2\rho V \omega_{\beta}}} \left(\overline{\beta} \cdot \overline{\epsilon}_{\beta}\right) D_{A} \left(\left\langle \psi_{nk'} \right| e^{i\beta \cdot r} \right| \psi_{nk} \right) \sqrt{n_{\beta}} + \left\langle \psi_{nk'} \right| e^{-i\beta \cdot r} \left| \psi_{nk} \right\rangle \sqrt{n_{\beta} + 1} \right)$$
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
OverviewStep 1: Determine Scattering Potential $U_{e-ph} = \sum_{\beta} D_A (\overline{\beta} \cdot \overline{\epsilon}_{\beta}) \sqrt{\frac{\overline{h}}{2\rho V \omega_{\beta}}} (\widehat{a}_{\beta} e^{i(\beta r - \omega t)} + \widehat{a}_{\beta}^{\dagger} e^{-i(\beta r - \omega t)})$ Step 2: Calculate Matrix Elements $H_{kk'} = \sum_{\beta} \sqrt{\frac{\overline{h}}{2\rho V \omega_{\beta}}} (\overline{\beta} \cdot \overline{\epsilon}_{\beta}) D_A (\sqrt{n_{\beta}} \ \delta_{k'=k+\beta} + \sqrt{n_{\beta}+1} \ \delta_{k'=k-\beta})$ Step 3: Calculate State-State Transition RatesStep 4: Calculate State LifetimeStep 5: Calculate Ensemble Lifetime

Electron-Phonon Scattering Rate

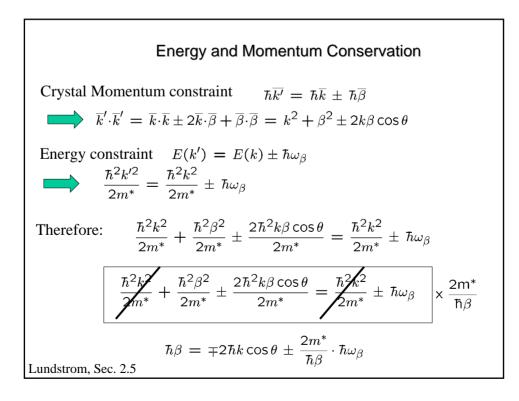
$$|H_{kk'}^{a}|^{2} = \frac{\hbar}{2\rho V \omega_{\beta}} \beta^{2} D_{A}^{2} n_{\beta} \delta_{k'=k+\beta}$$

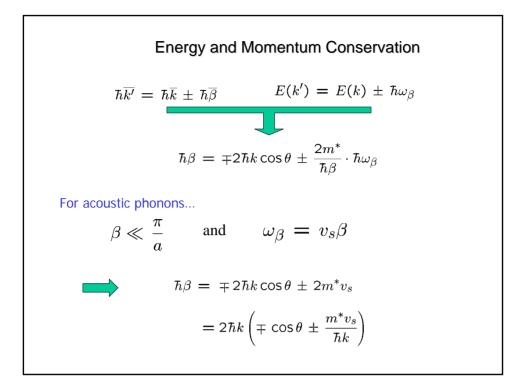
$$|H_{kk'}^{a}|^{2} = \frac{\hbar}{2\rho V \omega_{\beta}} \beta^{2} D_{A}^{2} (n_{\beta}+1) \delta_{k'=k-\beta}$$

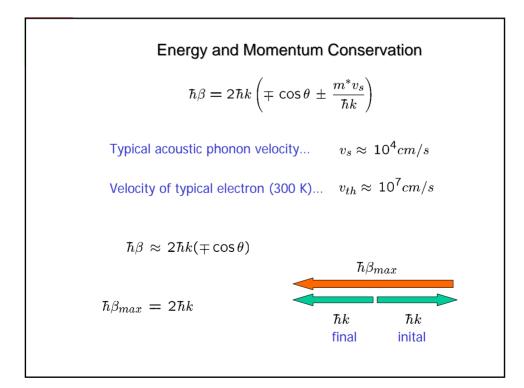
$$S(k,k') = \frac{\pi}{\rho V \omega_{\beta}} \beta^{2} D_{A}^{2} n_{\beta} \delta_{k'=k+\beta} \delta \left(E(k') - E(k) - \hbar \omega_{\beta} \right)$$

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

Scattering Rate Calculations Overview Step 1: Determine Scattering Potential $U_{e-ph} = \sum_{\beta} D_A \left(\overline{\beta} \cdot \overline{\epsilon}_{\beta}\right) \sqrt{\frac{\hbar}{2\rho V \omega_{\beta}}} \left(\hat{a}_{\beta} e^{i(\beta r - \omega t)} + \hat{a}^{\dagger}_{\beta} e^{-i(\beta r - \omega t)}\right)$ 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

Maximum momentum exchange...

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

Maximum energy exchange...

$$\begin{split} \hbar\omega_{\beta_{max}} &= \hbar\beta_{max}v_s \approx 2 \cdot (m^*v_{th})v_s \\ &\approx 2\left(\frac{1}{20} \cdot 10^{-30}[kg] \cdot 10^7[cm/s]\right) 10^5[cm/s] \\ &\approx 2\left(\frac{1}{20} \cdot 10^{-30}[kg] \cdot 10^5[m/s]\right) 10^3[m/s] \\ &\approx 10^{-4}[eV] = 0.1[meV] \end{split}$$

Acoustic phonon scattering is essentially elastic for 300K electrons...

Scattering Rate Calculations
Overview
Step 1: Determine Scattering Potential

$$U_{e-ph} = \sum_{\beta} D_A (\overline{\beta} \cdot \overline{\epsilon}_{\beta}) \sqrt{\frac{\overline{h}}{2\rho V \omega_{\beta}}} (\hat{a}_{\beta} e^{i(\beta r - \omega t)} + \hat{a}_{\beta}^{\dagger} e^{-i(\beta r - \omega t)})$$
Step 2: Calculate Matrix Elements

$$H_{kk'} = \sum_{\beta} \sqrt{\frac{\overline{h}}{2\rho V \omega_{\beta}}} (\overline{\beta} \cdot \overline{\epsilon}_{\beta}) D_A (\sqrt{n_{\beta}} \delta_{k'=k+\beta} + \sqrt{n_{\beta}+1} \delta_{k'=k-\beta})$$
Step 3: Calculate State-State Transition Rates

$$S(k, k') = \frac{\pi}{\rho V \omega_{\beta}} \beta^2 D_A^2 n_{\beta} \delta_{k'=k+\beta} \delta (E(k') - E(k) - \overline{h} \omega_{\beta}) + \frac{\pi}{\rho V \omega_{\beta}} \beta^2 D_A^2 (n_{\beta}+1) \delta_{k'=k-\beta} \delta (E(k') - E(k) + \overline{h} \omega_{\beta})$$
Step 4: Calculate State Lifetime

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

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

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

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