ECE 656: Electronic Transport in Semiconductors Fall 2017

Acoustic Phonon Scattering

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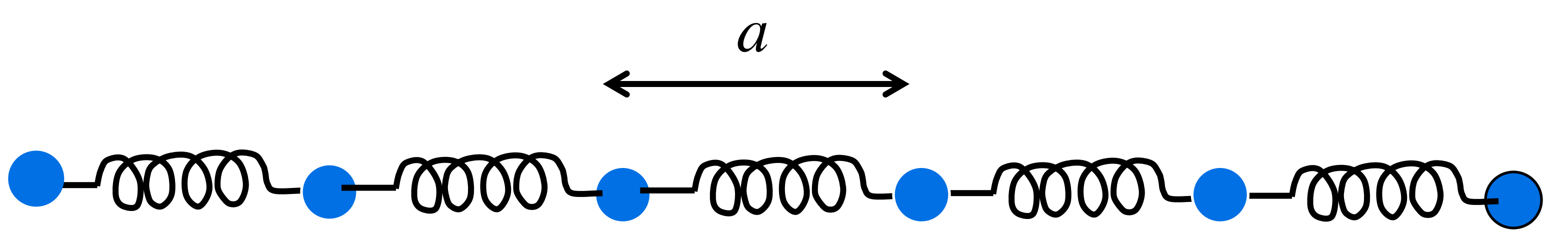
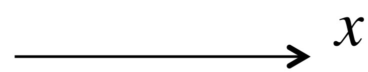
Outline

1) Quick review of acoustic phonons
2) Electron-phonon coupling (ADP)
3) Phonon amplitude
4) Matrix element and transition rate
5) Momentum and energy conservation
6) Scattering time
7) Summary

Lattice vibrations



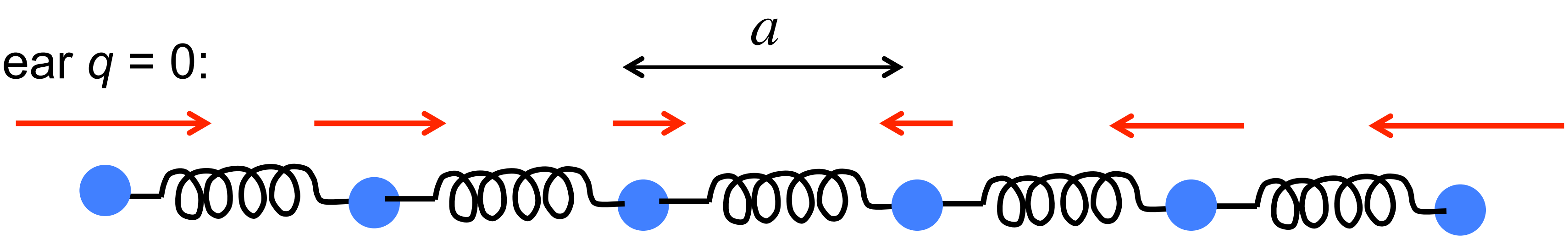
$$\vec{u}(x) = A_q \hat{e}_\nu e^{i(qx-\omega t)}$$



$\hat{e}_\nu = \hat{x}$	longitudinal
$\hat{e}_\nu = \hat{y}$	transverse
$\hat{e}_\nu = \hat{z}$	transverse

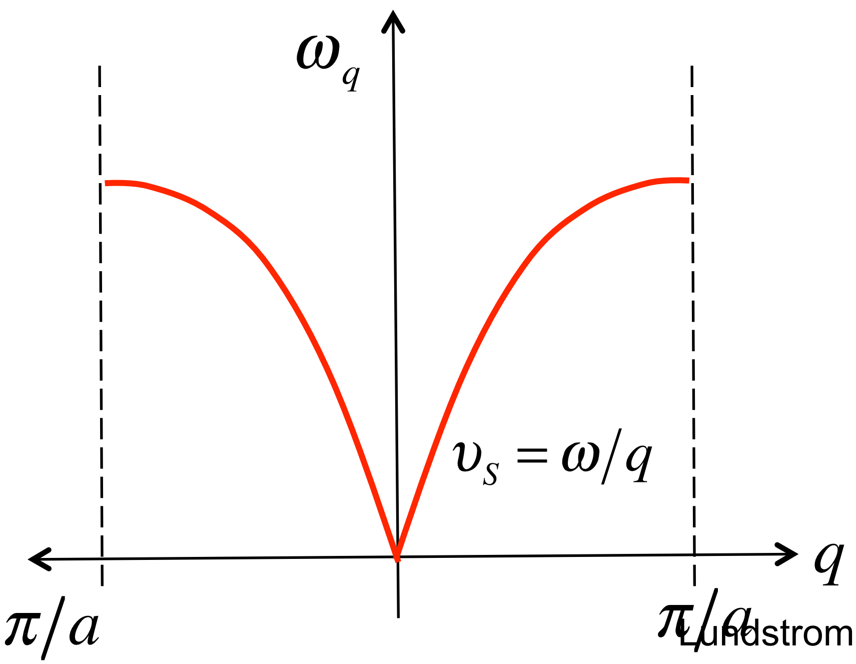
LA phonons

near $q = 0$:



$$\vec{u}(x) = A_q \, \hat{e}_\nu \, e^{i(qx - \omega t)}$$

$\longrightarrow x$



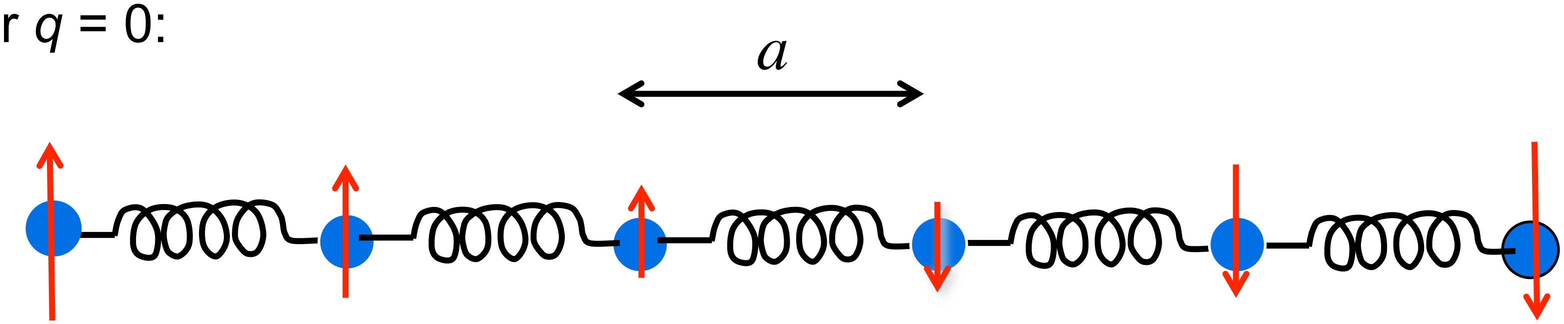
$\omega(q)$ dispersion

$$\omega/q = \upsilon_S = \sqrt{c_\ell/\rho} \approx 8.433 \times 10^5 \text{ cm/s}$$

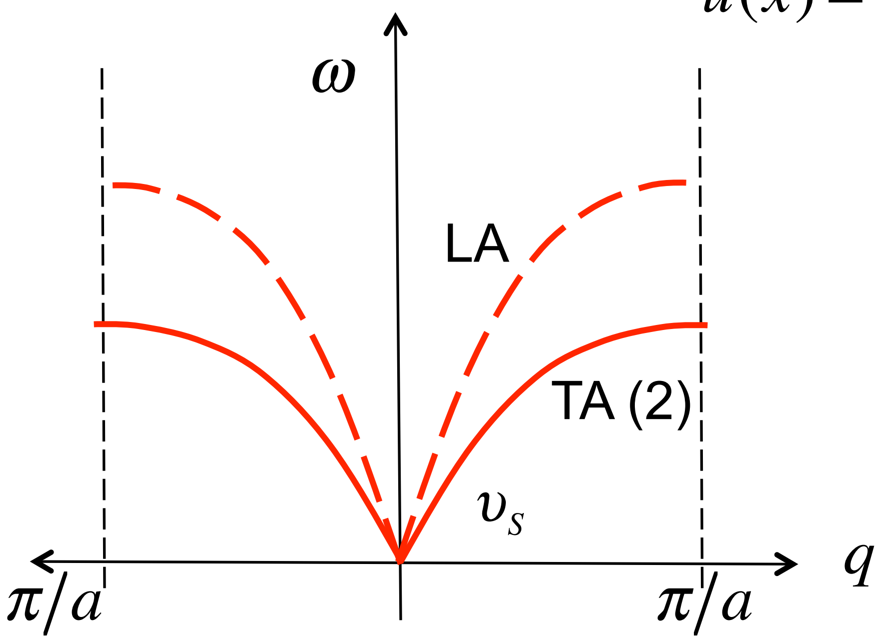
(silicon)

TA phonons

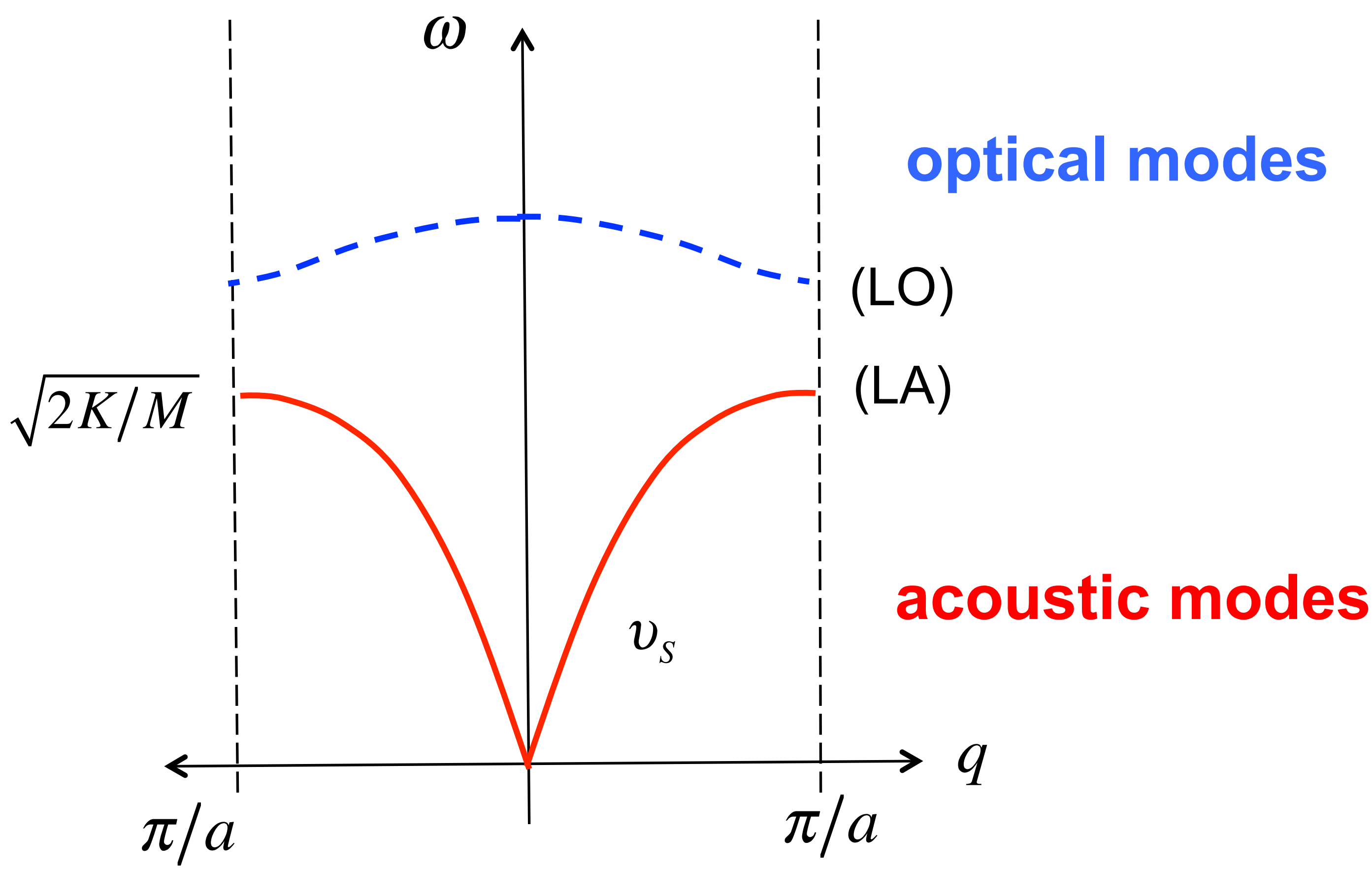
near $q = 0$:



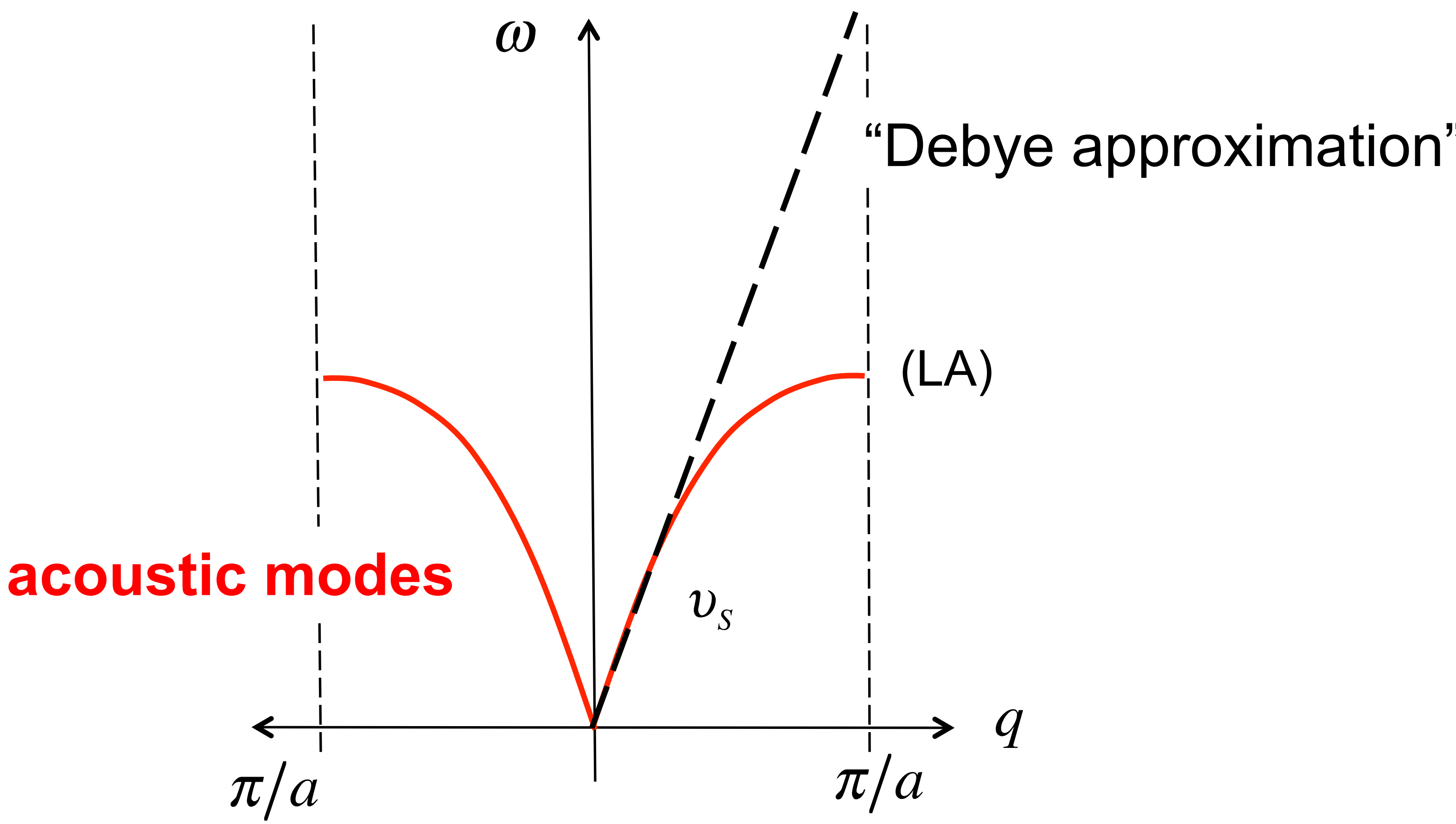
$$\vec{u}(x) = A_q \, \hat{e}_\nu \, e^{i(qx - \omega t)}$$



1D spring model (longitudinal modes)



Simplified dispersion for acoustic phonons



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Electron-phonon coupling (LA)

The bandgap depends on lattice constant: $\delta E_G = D\frac{\delta a}{a}$

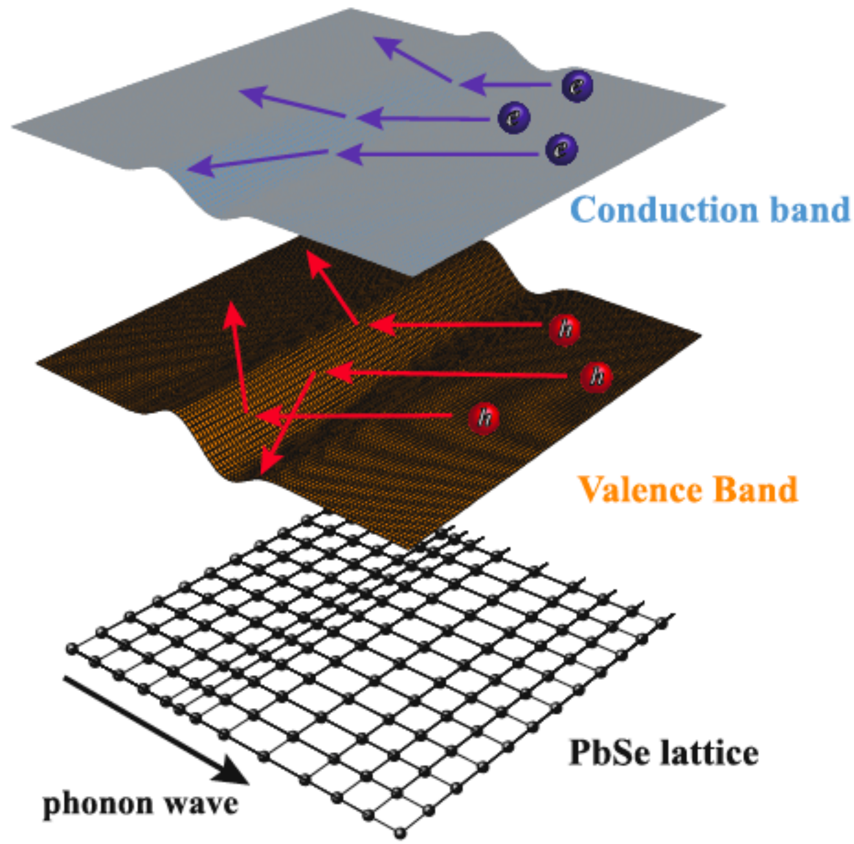
$\delta E_C = D_C\frac{\delta a}{a}$ "deformation potential"

Acoustic deformation potential (ADP) scattering

Physical picture

Carrier-phonon interaction via deformation potential scattering. Lattice deformed by phonon waves produces potential energy fluctuations in each band, resulting in scattering of carriers.

In PbSe, the fluctuation is smaller in the conduction band than in the valence band, so the electron mobility is higher than that of holes

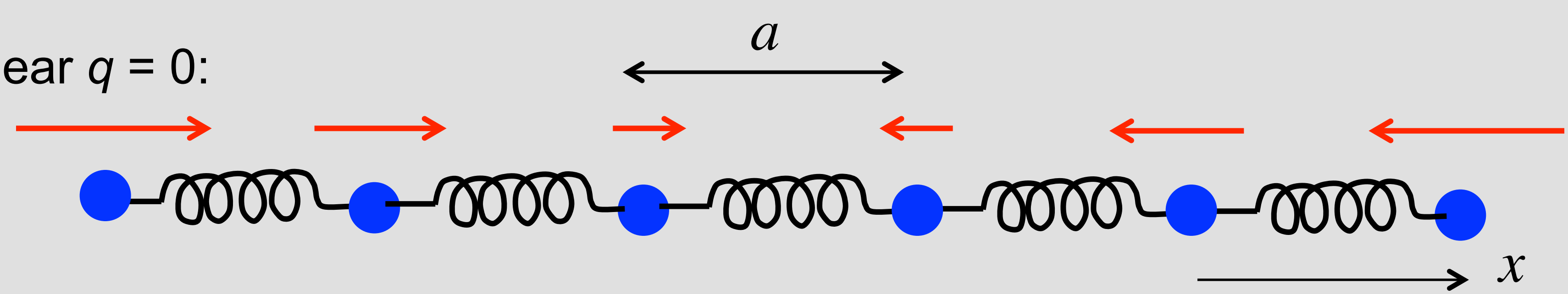


H. Wang, Y. Pei, A.D. LaLonde, and G. J. Snyder, “Material Design Considerations based on Thermoelectric Quality Factor,” Chapter 1 in Thermoelectric Nanomaterials, (K. Koumoto and T. Mori, editors), Springer-Verlag, 2013.

Electron-phonon coupling (LA)

LA phonons:

near q = 0:



$$\delta a = u(x) - u(x-a) = u(x) - \left\{ u(x) - \frac{\partial u}{\partial x} a \right\} = \frac{\partial u}{\partial x} a \qquad \frac{\delta a}{a} = \frac{\partial u}{\partial x}$$

"strain"

$$U_S = \delta E_C = D_C \frac{\delta a}{a}$$

Electron-phonon coupling

$$U_S = \delta E_C = D_C \frac{\delta a}{a} = D_C \frac{\partial u_q}{\partial x}$$

$$u_q(x,t) = A_q e^{\pm i(qx - \omega t)}$$

$$U_S = D_A \frac{\partial u_q}{\partial x} = \pm iqD_A u_q = K_q u_q$$

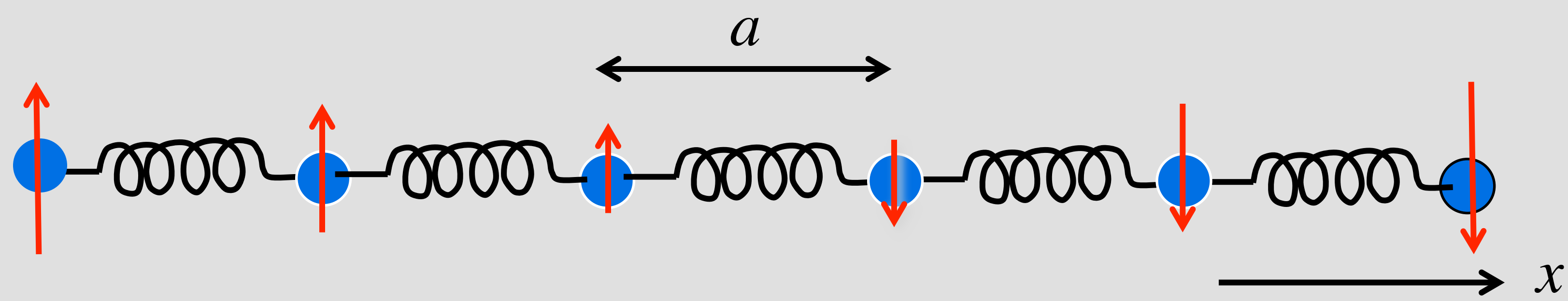
$$|K_q|^2 = q^2 D_A^2$$

"acoustic deformation potential (ADP) scattering"

Electron-phonon scattering (TA)

bandgap depends on lattice constant: $\delta E_G = D\dfrac{\delta a}{a}$

near β = 0:

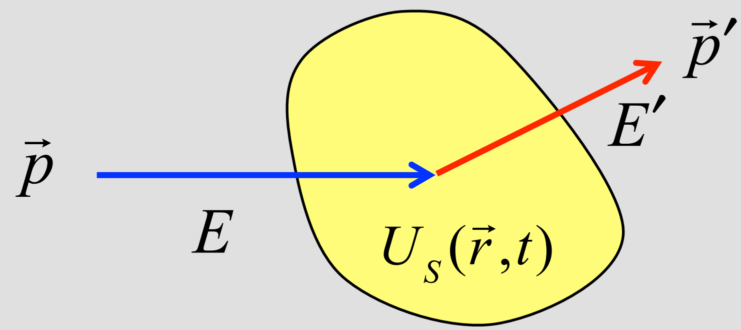


$$\frac{\delta a}{a} \propto \left(\frac{\partial u}{\partial x}\right)^2$$

To first order, ***only*** LA phonons scatter electrons

Recall: Oscillating potential

$$\psi_i = \frac{1}{\sqrt{\Omega}} e^{i\vec{p}\bullet\vec{r}/\hbar}$$



$$\psi_f = \frac{1}{\sqrt{\Omega}} e^{i\vec{p}'\bullet\vec{r}/\hbar}$$

$$U_S(\vec{r},t) = U_q^{a,e} e^{\pm i(\vec{q}\bullet\vec{r}-\omega t)}$$

$$u(\vec{r},t) = A_q^{a,e} e^{\pm i(\vec{q}\bullet\vec{r}-\omega t)}$$

$$S(\vec{p},\vec{p}') = \frac{2\pi}{\hbar}\left|H_{\vec{p}',\vec{p}}\right|^2 \delta\left(E' - E \mp \Delta E\right) \qquad H_{p',p} = U_q^{a,e}\delta\left(p' - \vec{p} \mp \hbar\vec{q}\right)$$

$$S(\vec{p},\vec{p}') = \frac{2\pi}{\hbar}\left|U_q^{a,e}\right|^2 \delta\left(p' - \vec{p} \mp \hbar\vec{q}\right)\delta\left(E' - E \mp \Delta E\right)$$

$$\left|U_q^{a,e}\right|^2 = \left|K_q\right|^2 \left|A_q^{a,e}\right|^2 \qquad \left|K_q\right|^2 = q^2 D_A^2 \qquad \left|A_q\right|^2 = ?$$

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Phonon amplitude

$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|K_q\right|^2\left|A_q^{a,e}\right|^2\delta\left(p' - \vec{p} \mp \hbar\vec{q}\right)\delta\left(E' - E \mp \Delta E\right)$$

$$u_q(\vec{r},t) = A_q e^{\pm i(\vec{q}\bullet\vec{r} - \omega t)} \qquad u_q(t) = A_q e^{-i\omega t} + A_q^* e^{i\omega t} \qquad u_q(t) = 2\left|A_q\right|\cos(\omega t + \phi)$$

$$\omega = \sqrt{K/M}$$

$$KE = \frac{1}{2}M\left(\frac{du}{dt}\right)^2 = \frac{1}{2}M\omega^2 4\left|A_q\right|^2 \sin^2(\omega t + \phi)$$

$$PE = \frac{1}{2}Ku^2 = \frac{1}{2}K4\left|A_q\right|^2\cos^2(\omega t + \phi) = \frac{1}{2}M\omega^2 4\left|A_q\right|^2\cos^2(\omega t + \phi)$$

$$E = KE + PE = 2M\omega^2\left|A_q\right|^2$$

$$E = \left(N_\omega + \frac{1}{2}\right)\hbar\omega$$

$$\left|A_\beta\right|^2 \to \frac{\hbar\omega}{2M\omega^2}\left(N_\omega + \frac{1}{2}\right)$$

(almost)

S. Datta, *Atom to Transistor*, Sec. 10.4

Absorption vs. emission

$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|K_q\right|^2\left|A_q^{a,e}\right|^2 \delta\left(p' - \vec{p} \mp \hbar\vec{q}\right)\delta\left(E' - E \mp \Delta E\right)$$

$$\left|A_\beta\right|^2 \rightarrow \frac{\hbar\omega}{2M\omega^2}\left(N_\omega + \frac{1}{2}\right) = \frac{\hbar}{2\rho\Omega\omega}\left(N_\omega + \frac{1}{2}\right)$$ (almost)

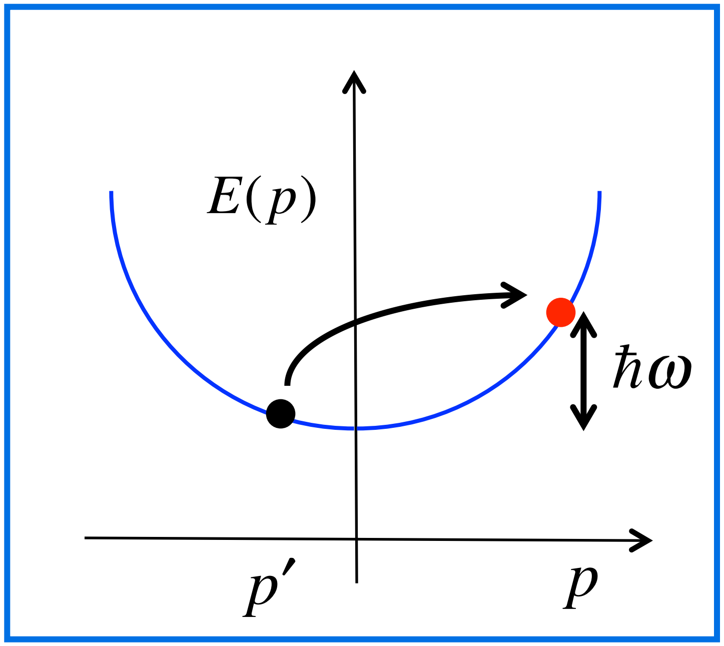
We can show that:

$$S^{ABS}(\vec{p}\,',\vec{p}) \sim N_\omega$$

$$S^{EMS}(\vec{p},\vec{p}\,') \sim N_\omega + 1$$

$$N_\omega = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$

Absorption vs. emission

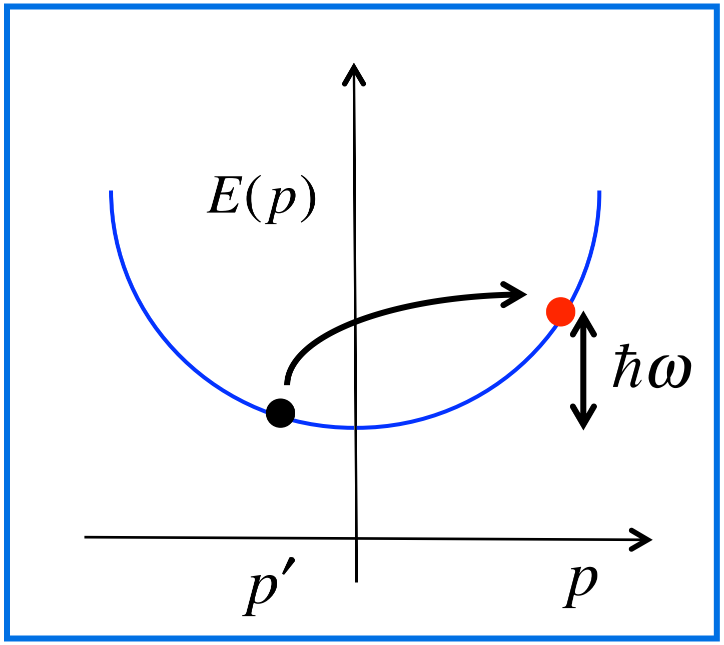


$$\frac{S^{ABS}(\vec{p}',\vec{p})}{S^{EMS}(\vec{p},p')} = e^{-\hbar\omega/k_B T}$$

$$S^{ABS}(\vec{p}',\vec{p})f_0(E')\left[1-f_0(E)\right] = S^{EMS}(\vec{p},\vec{p}')f_0(E)\left[1-f_0(E')\right]$$

$$f_0(E) = \frac{1}{1+e^{(E-E_F)/k_B T}}$$

Absorption vs. emission



$$\frac{S^{ABS}(\vec{p}',\vec{p})}{S^{EMS}(\vec{p},p')} = e^{-\hbar\omega/k_B T}$$

$$S^{ABS}(\vec{p}',\vec{p}) \sim N_\omega$$

$$S^{EMS}(\vec{p},\vec{p}') \sim N_\omega + 1$$

$$N_\omega = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$

$$\left|A_\beta^{ABS}\right|^2 \rightarrow \frac{\hbar}{2\rho\Omega\omega} N_\omega$$

$$\left|A_\beta^{EMS}\right|^2 \rightarrow \frac{\hbar}{2\rho\Omega\omega} (N_\omega + 1)$$

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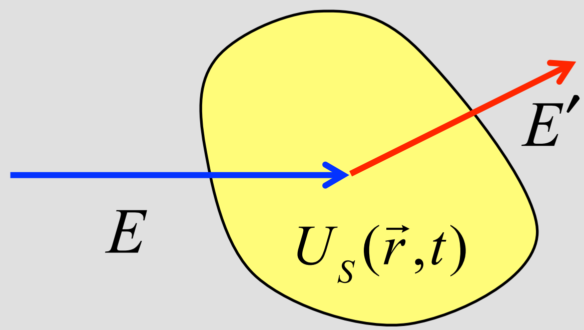
ADP Phonon scattering

$$\psi_i = \frac{1}{\sqrt{\Omega}} e^{i\vec{p}\bullet\vec{r}/\hbar} \qquad \vec{p}$$



$$\vec{p}' \qquad \psi_f = \frac{1}{\sqrt{\Omega}} e^{i\vec{p}'\bullet\vec{r}/\hbar}$$

$$U_S\left(\vec{r},t\right) = U_q^{a,e} e^{\pm i\left(\vec{q}\bullet\vec{r}-\omega t\right)}$$

$$S\left(\vec{p},\vec{p}'\right) = \frac{2\pi}{\hbar}\left|U_q^{a,e}\right|^2 \delta\left(p' - \vec{p} \mp \hbar\vec{q}\right)\delta\left(E' - E \mp \Delta E\right)$$

$$\left|U_q^{a,e}\right|^2 = \left|K_q^{a,e}\right|^2 \left|A_q^{a,e}\right|^2 = q^2 D_A^2 \left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)\frac{\hbar}{2\Omega\rho\omega_q}$$

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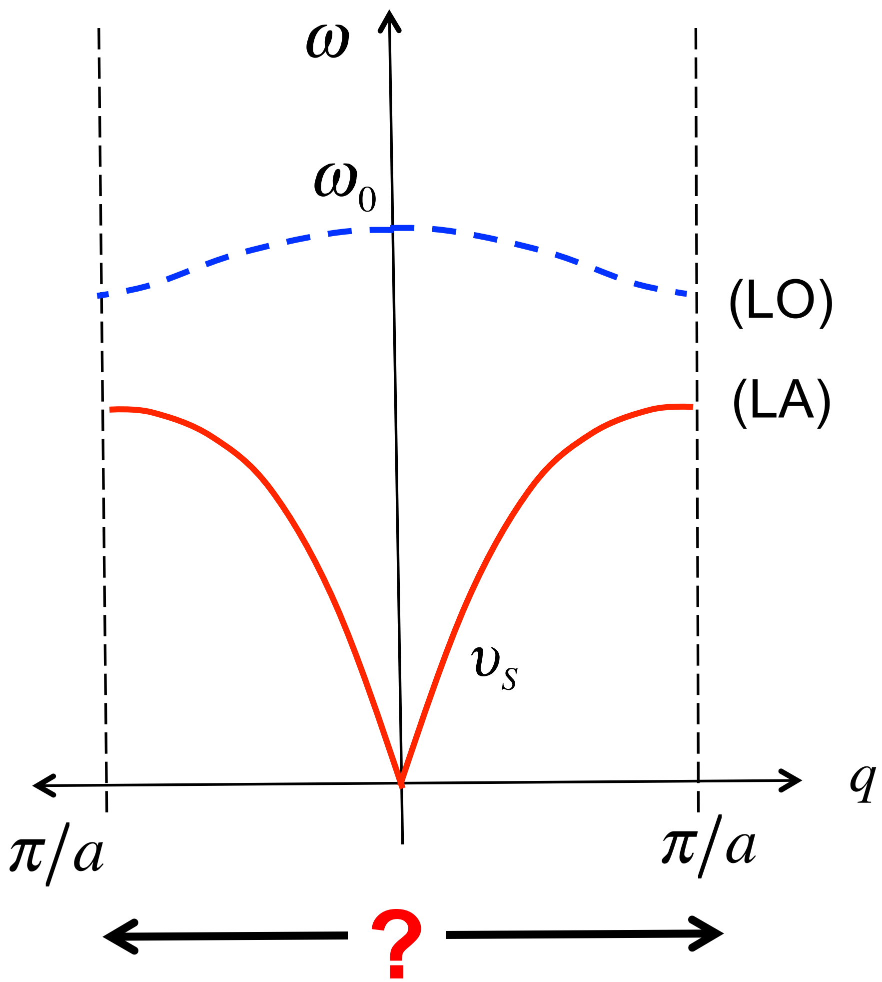
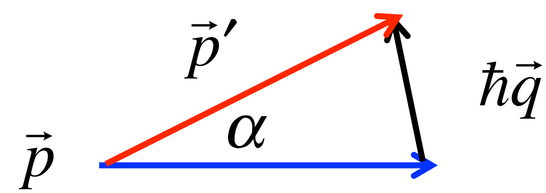
Which phonons scatter?





$$E' = E \pm \hbar\omega_q$$

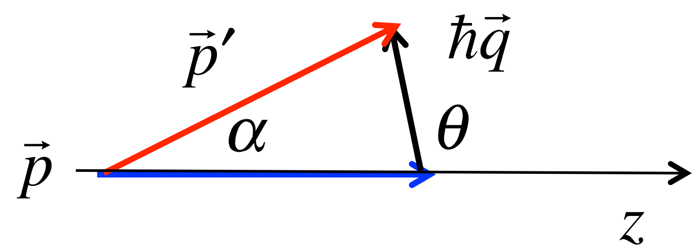
$$\vec{p}\,' = \vec{p} \pm \hbar\vec{q}$$

Momentum conservation

$$\frac{p'^2}{2m^*} = \frac{p^2}{2m^*} \pm \hbar\omega_q$$

$$\vec{p}' = \vec{p} \pm \hbar\vec{q}$$

intravalley
scattering



$$\vec{p}' \bullet \vec{p}' = \left(\vec{p} \pm \hbar\vec{q}\right) \bullet \left(\vec{p} \pm \hbar\vec{q}\right)$$

$$p'^2 = p^2 \pm 2\hbar\,\vec{p} \bullet \vec{q} + \hbar^2 q^2$$

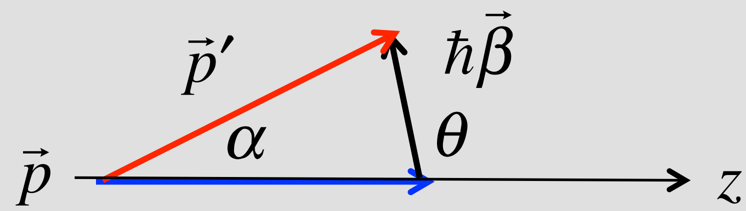
$$\pm\hbar\omega_q = \pm\hbar\frac{\vec{p} \bullet \vec{q}}{m^*} + \frac{\hbar^2 q^2}{2m^*}$$

$$\hbar q = 2p\left[\mp\cos\theta \pm \frac{\omega_q}{q\upsilon}\right]$$

top sign: ABS
bottom sign: EMS

Maximum q: acoustic phonons

$$\hbar q = 2p\left[\mp\cos\theta \pm \frac{\omega_q}{q\upsilon}\right]$$



$$\hbar q_{\max} = 2p\left[1 \pm \frac{\omega_q}{q_{\max}\upsilon}\right] \qquad \omega_q = \upsilon_S q \qquad \hbar q_{\max} = 2p\left[1 \pm \frac{\upsilon_S}{\upsilon}\right]$$

To emit an AP, the electron's velocity must be greater than the phonon's.

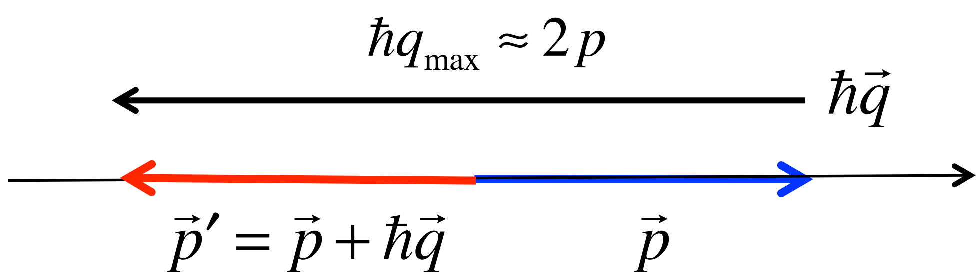
$$\upsilon_S < 10^6 \text{ cm/s}$$

$$\langle \upsilon \rangle \approx 10^7 \text{ cm/s}$$

$$\hbar q_{\max} \approx 2p$$

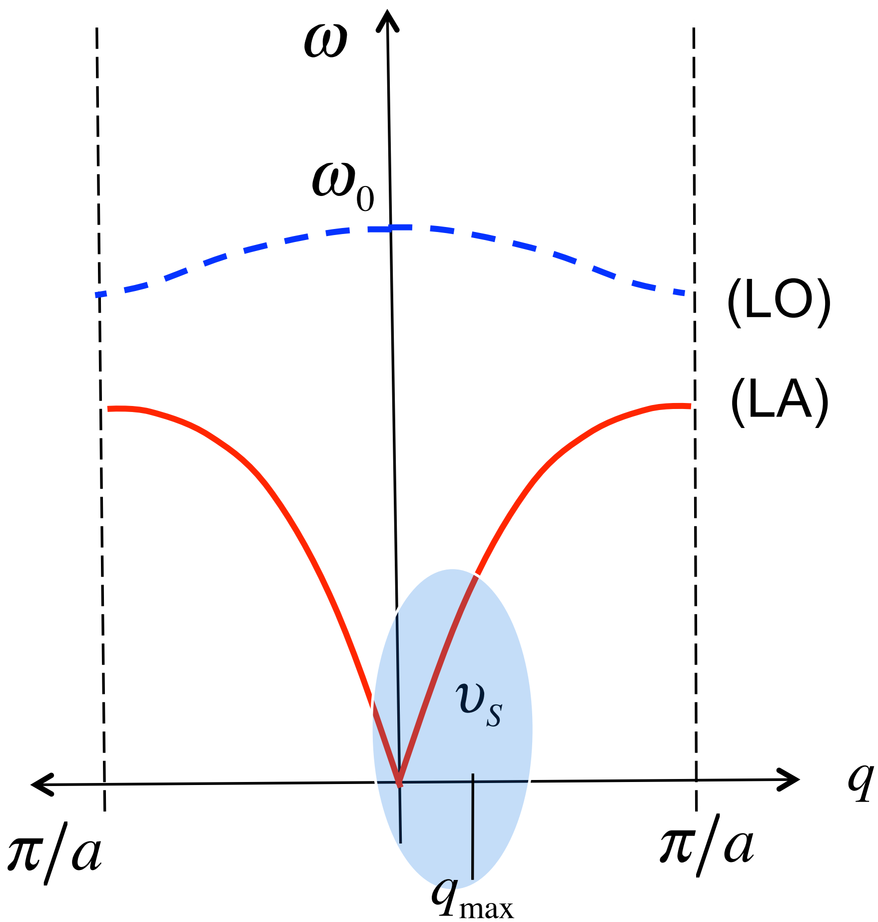
Maximum q: acoustic phonons

$$\hbar q_{\max} = 2p\left[1 \pm \frac{\upsilon_S}{\upsilon}\right] \qquad \upsilon_S < 10^6 \text{ cm/s} \qquad \langle \upsilon \rangle \approx 10^7 \text{ cm/s}$$



Near room temperature, intra-valley acoustic phonon scattering is nearly elastic.

Maximum q: Acoustic phonons



$$\hbar q_{max} \approx 2p$$

$$\frac{q_{max}}{\pi/a} = \frac{2p}{\hbar \pi/a} \approx \frac{1}{4}$$

$$\left(p = m_0 \upsilon, a = 5 \text{ Ang}\right)$$

$$\Delta E_{max} = \hbar\omega_{max} = \hbar q_{max}\upsilon_S \approx 10^{-3}\text{ eV}$$

Acoustic phonon scattering is nearly elastic (at room temperature) and involves phonons near the zone center.

Summary

1) Energy-momentum conservation restrict the range of phonon wavevectors that can scatter electrons.

$$q_{\min} < \beta < q_{\max}$$

2) Intra-valley acoustic phonon scattering is approximately elastic at room temperature.

$$0 < \hbar q < 2p$$

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Scattering times

$$S(\vec{p},\vec{p}') = \frac{2\pi}{\hbar}\left|K_q^{a,e}\right|^2\left|A_q^{a,e}\right|^2 \delta\left(p' - \vec{p} \mp \hbar\vec{q}\right)\delta\left(E' - E \mp \hbar\omega\right)$$

$$\left|K_q^{a,e}\right| = q^2 D_A^2 \qquad \left|A_q^{a,e}\right|^2 = \left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)\frac{\hbar}{2\Omega\rho\omega_q}$$

$$\frac{1}{\tau(\vec{p})} == \sum_{\vec{p}',\uparrow} S(\vec{p},\vec{p}') \qquad \frac{1}{\tau_m(\vec{p})} = \sum_{\vec{p}',\uparrow} S(\vec{p},\vec{p}')\frac{\Delta p_z}{p_{z0}}$$

Energy-momentum conservation

$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|K_q^{a,e}\right|^2\left|A_q^{a,e}\right|^2 \delta\left(p' - \vec{p} \mp \hbar\vec{q}\right)\delta\left(E' - E \mp \hbar\omega\right)$$

Energy and momentum conservation:

$$\vec{p}\,' = \vec{p} \pm \hbar\vec{\beta} \qquad E' = E \pm \mathrm{h}\omega_\beta$$

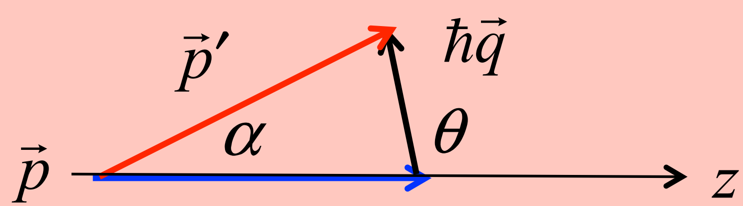
$$\delta\left(p' - \vec{p} \mp \hbar\vec{q}\right)\delta\left(E' - E \mp \hbar\omega\right) \rightarrow \frac{1}{\hbar\upsilon q}\delta\left(\pm\cos\theta + \frac{\hbar q}{2p} \mp \frac{\omega_q}{\upsilon q}\right)$$

Transition rate

$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|K_q\right|^2 \frac{\hbar}{2\rho\Omega\omega}\frac{1}{\hbar\upsilon q}\left(N_q + \frac{1}{2} \mp \frac{1}{2}\right)\delta\left(\pm\cos\theta + \frac{\hbar q}{2p} \mp \frac{\omega}{\upsilon q}\right)$$

$$S(\vec{p},\vec{p}\,') = \frac{1}{\Omega}C_q\left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)\delta\left(\pm\cos\theta + \frac{\hbar q}{2p} \mp \frac{\omega}{\upsilon q}\right)$$

$$C_q = \frac{\pi}{\hbar\rho\upsilon\omega q}\left|K_q\right|^2 \qquad N_\omega = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$



General expression for scattering time

$$\frac{1}{\tau} = \sum_{\vec{p}',\uparrow} S(\vec{p},\vec{p}') = \sum_{\vec{q},\uparrow} S(\vec{p},\vec{p}') \qquad \vec{p}' = \vec{p} \pm \hbar\vec{q}$$

Integration of the delta function simply restricts *q* to those values that satisfy energy and momentum conservation.

$$q_{\min} < q < q_{\max}$$

$$\frac{1}{\tau} = \frac{1}{4\pi^2} \int_{q_{\min}}^{q_{\max}} C_q \left(N_\omega + \frac{1}{2} \mp \frac{1}{2} \right) q^2 \, dq$$

$$C_q = \frac{\pi}{\hbar \rho \upsilon \omega q} \left| K_q \right|^2 \qquad N_\omega = \frac{1}{e^{\hbar\omega / k_B T} - 1}$$

Simpler approach

$$S(\vec{p},\vec{p}') = \frac{2\pi}{\hbar}\left|K_q^{a,e}\right|^2\left|A_q^{a,e}\right|^2 \delta\left(p' - \vec{p} \mp \hbar\vec{q}\right)\delta\left(E' - E \mp \hbar\omega\right)$$

If there is no q dependence here, then the scattering is **isotropic**, and we don’t need to explicitly account for momentum conservation.

$$S(\vec{p},\vec{p}') = \frac{2\pi}{\hbar}\left|K_q^{a,e}\right|^2\left|A_q^{a,e}\right|^2 \delta\left(E' - E\right)$$

elastic

Simpler approach

$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|K_q^{a,e}\right|^2\left|A_q^{a,e}\right|^2\delta\left(E'-E\right)$$

$$\left|K_q^{a,e}\right| = q^2 D_A^2 \qquad \left|A_q^{a,e}\right|^2 = \left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)\frac{\hbar}{2\Omega\rho\,\omega_q}$$

$$N_\omega = \frac{1}{e^{\hbar\omega/k_B T}-1} \approx \frac{k_B T}{\hbar\omega} \qquad N_\omega \approx N_\omega + 1$$

“equipartition”

$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left\{q^2 D_A^2\right\}\left\{\left(\frac{k_B T}{\hbar\omega_q}\right)\frac{\hbar}{2\Omega\rho\,\omega_q}\right\}\delta\left(E'-E\right)$$

Simpler approach

$$S(\vec{p},\vec{p}')=\frac{2\pi}{\hbar}\left\{q^2D_A^2\right\}\left\{\left(\frac{k_BT}{\hbar\omega_q}\right)\frac{\hbar}{2\Omega\rho\,\omega_q}\right\}\delta\left(E'-E\right)$$

(absorption or emission)

$$\frac{\omega_q}{q}=\upsilon_S=\sqrt{\frac{c_\ell}{\rho}}$$

$$S(\vec{p},\vec{p}')=\frac{2\pi}{\hbar}\frac{D_A^2k_BT}{2c_\ell}\frac{1}{\Omega}\delta\left(E'-E\right)$$

Isotropic!

ADP scattering: 3D in a nutshell (iii)

$$S(\vec{p},\vec{p}') = \frac{2\pi}{\hbar} U_{ac} \frac{1}{\Omega} \delta(E' - E) \qquad U_{ac} = \frac{D_A^2 k_B T}{2c_l}$$

(abs or ems)

$$\frac{1}{\tau} = \frac{1}{\tau_m} = \sum_{\vec{p}'\uparrow} S(\vec{p},\vec{p}')$$

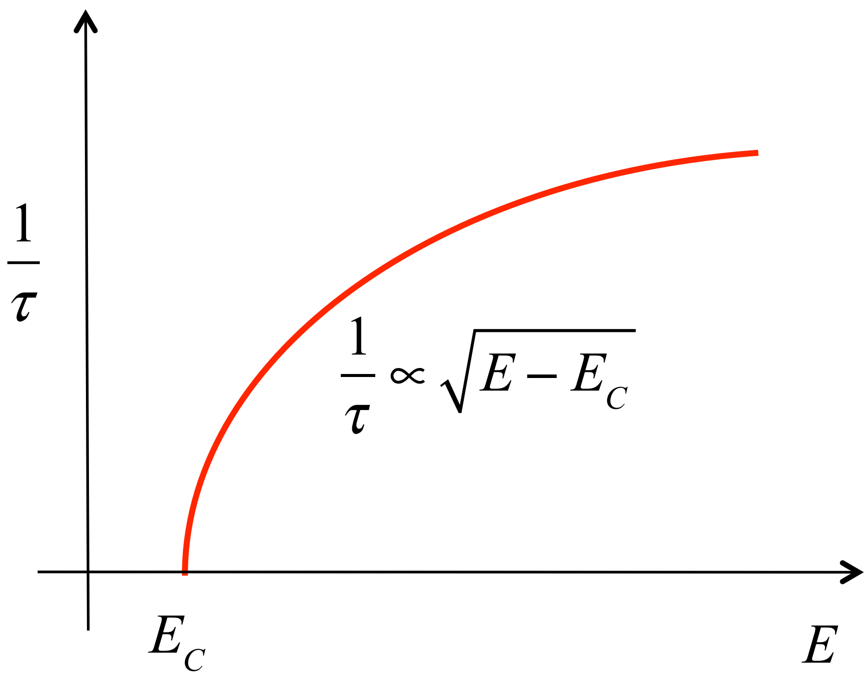
$$\frac{1}{\tau_{tot}} = \frac{1}{\tau_{abs}} + \frac{1}{\tau_{ems}} = \sum_{\vec{p}'} 2S(\vec{p},\vec{p}') = \frac{1}{\tau_m}$$

$$\frac{1}{\tau_m} = \frac{2\pi}{\hbar} U_{ac} \frac{D_{3D}(E)}{2} \times 2$$

ADP scattering: 3D in a nutshell (iii)

$$\frac{1}{\tau} = \frac{2\pi}{\hbar}\left(2U_{ac}\right)\frac{D_{3D}\left(E\right)}{2} = \frac{1}{\tau_m}$$

$$\tau = \tau_m = \frac{2c_l\hbar^4}{\pi D_A^2 m^* \sqrt{2m^*}}\frac{1}{\left(k_B T\right)}\frac{1}{\sqrt{E-E_C}}$$



"Power law scattering"

$$\tau = \tau_m = \tau_0\left(E/k_B T\right)^s$$

$$s = -1/2$$

$$\tau_0 = \frac{2c_l\hbar^4}{\pi D_A^2 m^* \sqrt{2m^*}}\frac{1}{\left(k_B T\right)^{3/2}}$$

Questions?

1) Quick review of acoustic phonons
2) Electron-phonon coupling (ADP)
3) Phonon amplitude
4) Matrix element and transition rate
5) Momentum and energy conservation
6) Scattering time
7) Summary