ECE 656: Electronic Transport in Semiconductors Fall 2017

Optical Phonon Scattering (ODP)

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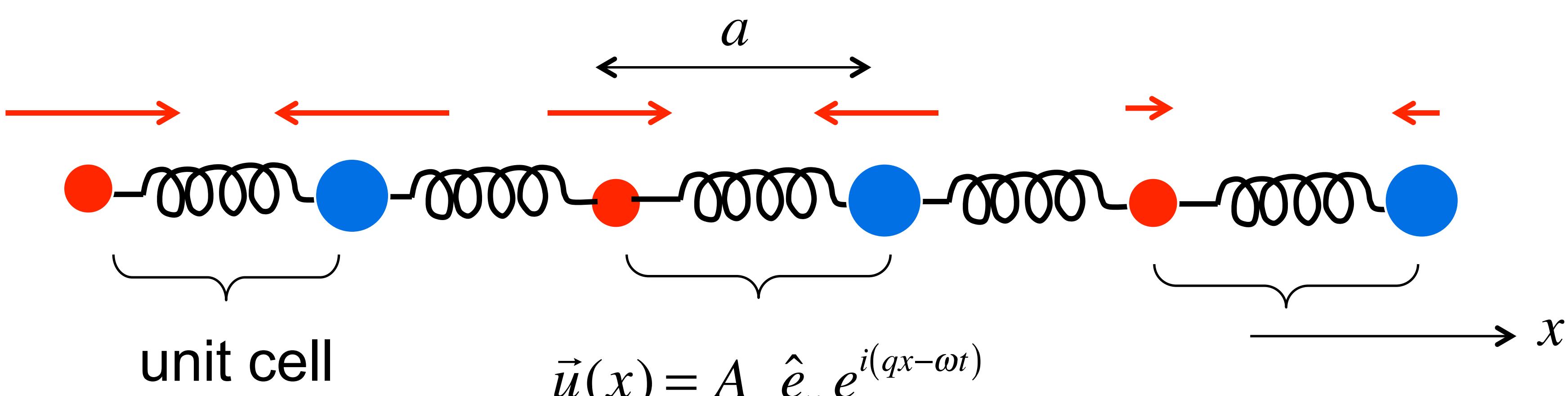
Outline

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

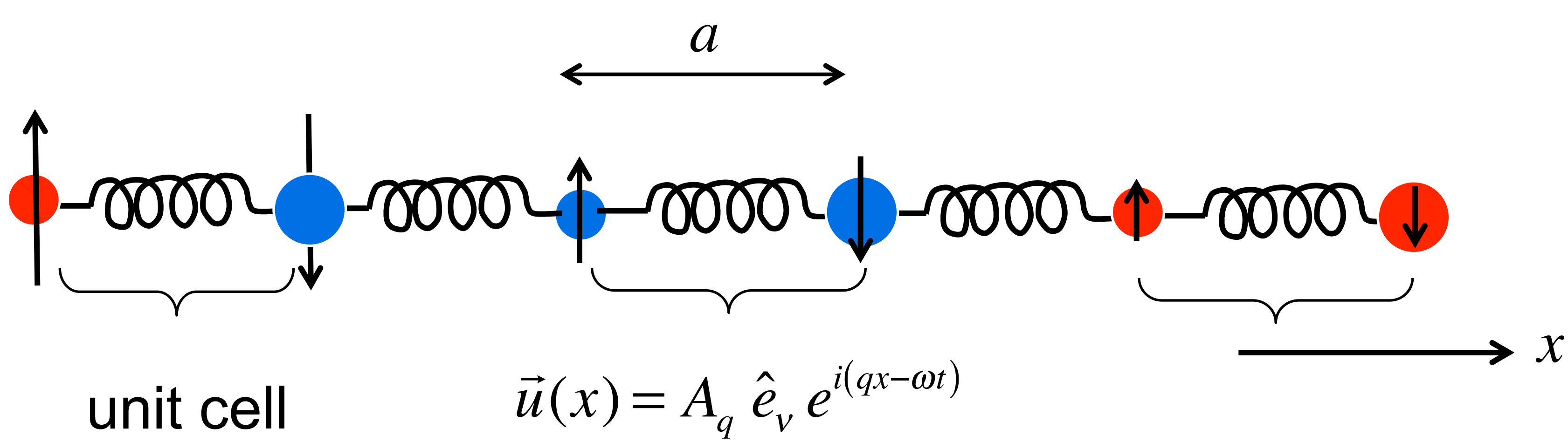
LO phonons



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

the two atoms in a unit cell oscillate out of phase

TO phonons

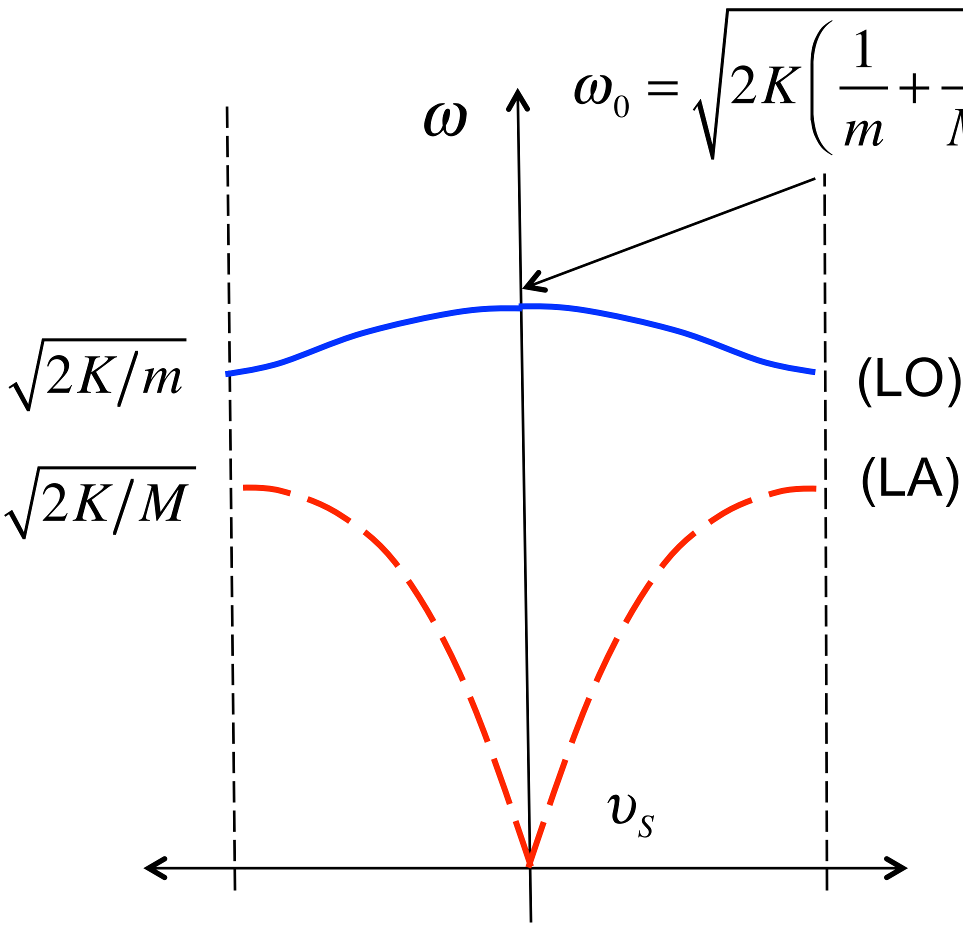


$$\vec{u}(x) = A_q \, \hat{e}_\nu \, e^{i(qx-\omega t)}$$

The two atoms in a unit cell oscillate out of phase

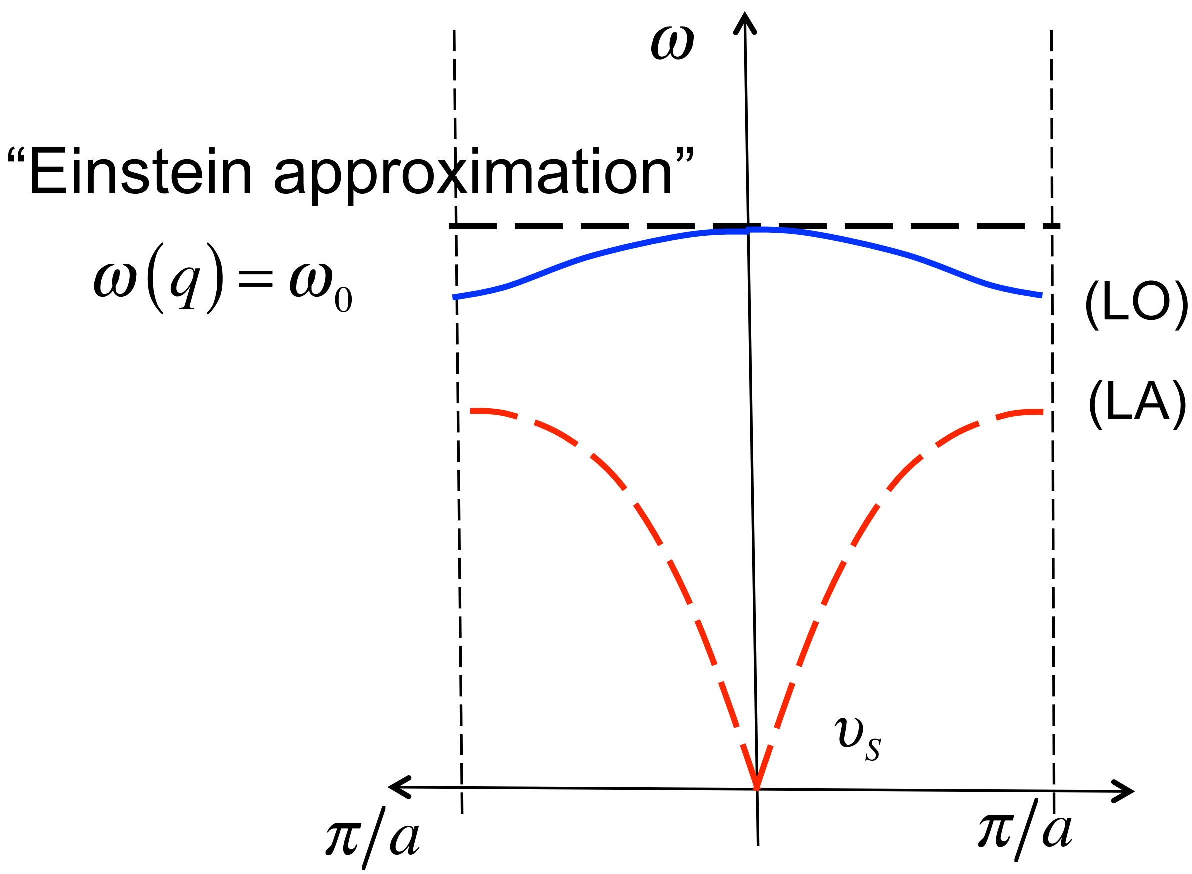
Coupling to electrons is not as strong as for LO phonons.

LO phonons



Optical phonons have **low group velocity**.

Simplified dispersion for optical phonons



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Electron-phonon coupling (LA)

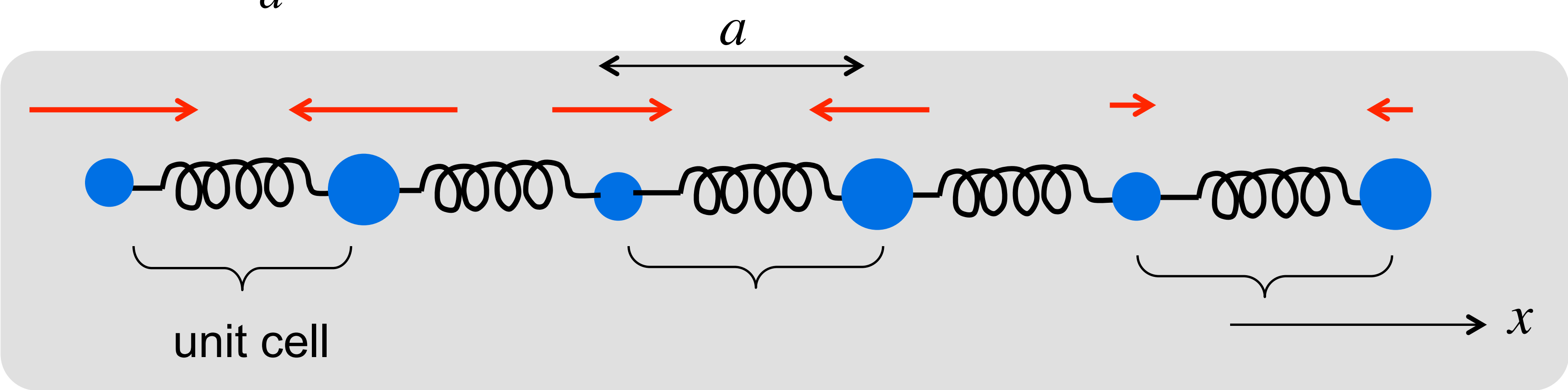
The bandgap depends on lattice constant: $\delta E_G = D\dfrac{\delta a}{a}$

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

Optical deformation potential (ODP) scattering

Electron-phonon coupling (LO)

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



$$\delta a(x) = u_q(x) \qquad u_q(x,t) = A_q e^{\pm i(qx - \omega t)} \qquad U_S \approx D_O u_q = K_q u_q$$

$$|K_q|^2 = D_O^2$$

"optical deformation potential scattering (ODP)"

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Phonon amplitude

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

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

$$\left|A_q^{a,e}\right|^2 \rightarrow \frac{\hbar}{2\rho\Omega\omega}\left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)$$

$$S^{abs}(\vec{p},\vec{p}') \propto N^\omega \qquad S^{ems}(\vec{p},\vec{p}') \propto N_\omega + 1$$

ABS EMS

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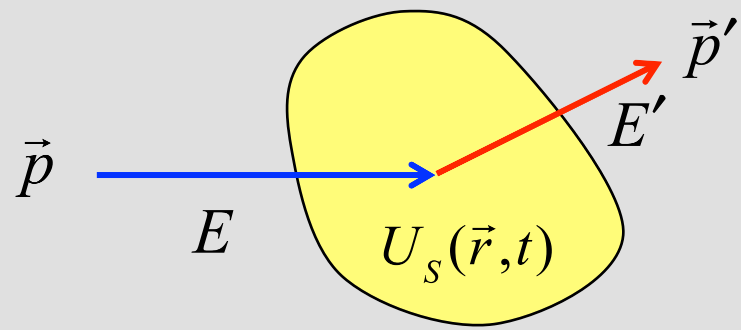
ODP Phonon scattering

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



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

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

$$S\left(\vec{p},\vec{p}\,'\right) = \frac{2\pi}{\hbar}\left|U_q^{a,e}\right|^2 \delta\left(p' - \vec{p} \mp \hbar\vec{q}\right)\delta\left(E' - E \mp \hbar\omega_0\right)$$

$$\left|U_q^{a,e}\right|^2 = \left|K_q^{a,e}\right|^2 \left|A_q^{a,e}\right|^2 = D_O^2\left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)\frac{\hbar}{2\Omega\rho\,\omega_0}$$

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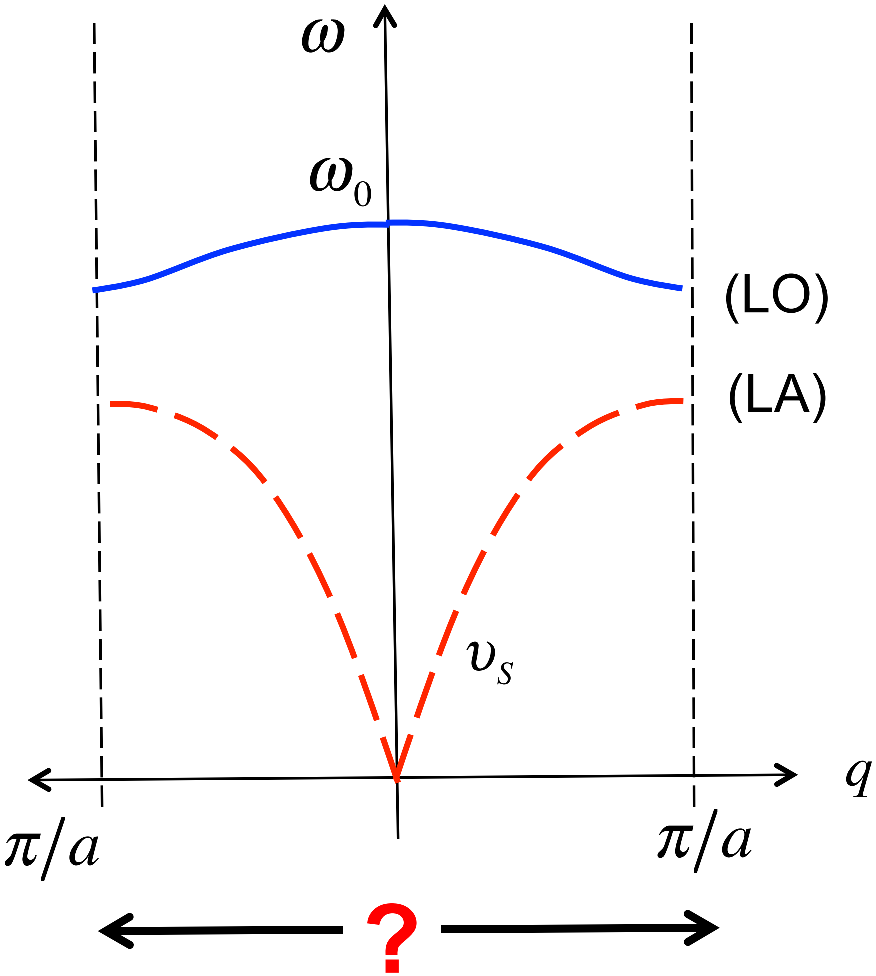
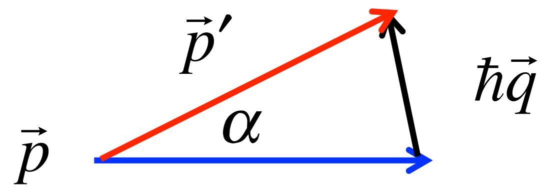
Which phonons scatter?





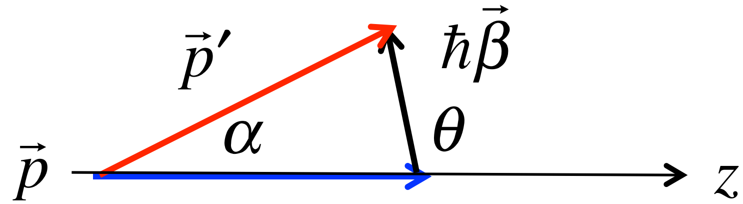
$$E' = E \pm \hbar\omega_0$$

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

Momentum conservation

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

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



$$\hbar q = 2p\left[\mp\cos\theta \pm \frac{\omega_0}{q\upsilon}\right]$$

top sign: ABS

$$\hbar q = 2p\left[\mp\cos\theta \pm \frac{\omega_0}{q\upsilon}\right]$$

$$\hbar q = p\left[-\cos\theta + \sqrt{\cos^2\theta \pm \frac{\hbar\omega_0}{E}}\right]$$

Any electron can absorb an optical phonon, but to emit an optical phonon, its energy must be > optical phonon energy.

$$\hbar q_{\max} = p\left[1 + \sqrt{1 \pm \frac{\hbar\omega_0}{E}}\right]$$

(inelastic)

Summary

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

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

2) Intra-valley optical phonon scattering is inelastic at room temperature and involves phonons near the zone center.

$$\hbar q_{\min} = p\left[\mp 1 \pm \left(1 \pm \hbar\omega_0 / E_k\right)^{1/2}\right] \qquad \text{(ABS/EMS)}$$

$$\hbar q_{\max} = p\left[1 + \left(1 \pm \hbar\omega_0 / E_k\right)^{1/2}\right] \qquad \text{(For EMS)} \quad E_k > \hbar\omega_0$$

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Scattering times

$$S(\vec{p},\vec{p}') = \frac{2\pi}{\hbar}\left|K_q^{a,e}\right|^2\left|A_q^{a,e}\right|^2\delta\left(p' - \vec{p} \mp \hbar\vec{q}\right)\delta\left(E' - E \mp \hbar\omega_0\right)$$

$$\left|K_q^{a,e}\right| = D_O^2 \qquad \left|A_q^{a,e}\right|^2 = \left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)\frac{\hbar}{2\Omega\rho\,\omega_0}$$

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

Simple approach

$$S(\vec{p},\vec{p}\,')=\frac{2\pi}{\hbar}\left|K_q^{a,e}\right|^2\left|A_q^{a,e}\right|^2\delta\left(p'-\vec{p}\mp\hbar\vec{q}\right)\delta\left(E'-E\mp\hbar\omega_0\right)$$

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

$$\frac{1}{\tau}=\frac{1}{\tau_m}$$

Simple approach

$$S(\vec{p},\vec{p}') = \frac{2\pi}{\hbar}\left|K_q^{a,e}\right|^2\left|A_q^{a,e}\right|^2\delta\left(E'-E\mp\hbar\omega_0\right)$$

$$\left|K_q^{a,e}\right| = D_O^2 \qquad \left|A_q^{a,e}\right|^2 = \left(N_\omega + \frac{1}{2}\mp\frac{1}{2}\right)\frac{\hbar}{2\Omega\rho\omega_0} \qquad N_\omega = \frac{1}{e^{\hbar\omega_0/k_BT}-1}$$

$$S(\vec{p},\vec{p}') = \frac{2\pi}{\hbar}D_O^2\frac{\hbar}{2\Omega\rho\omega_0}\left(N_\omega + \frac{1}{2}\mp\frac{1}{2}\right)\delta\left(E'-E\mp\hbar\omega_0\right)$$

ODP scattering

$$S\left(\vec{p},\vec{p}'\right)=\frac{2\pi}{\hbar}U_{op}^{a,e}\frac{1}{\Omega}\delta\left(E'-E\mp\hbar\omega_0\right) \qquad U_{op}^{a,e}=D_O^2\frac{\hbar}{2\Omega\rho\omega_0}\left(N_\omega+\frac{1}{2}\mp\frac{1}{2}\right)$$

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

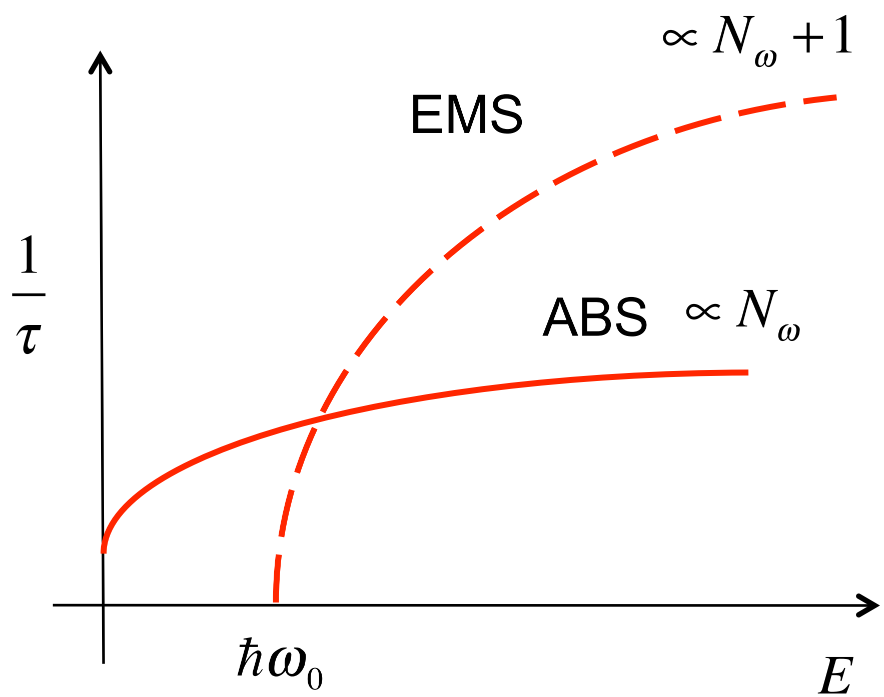
$$\frac{1}{\tau_m(E)}=\frac{2\pi}{\hbar}U_{op}^{a,e}\frac{D_{3D}\left(E\pm\hbar\omega_0\right)}{2}$$

$$\frac{1}{\tau_m^{abs}}\propto N_{\omega_0}$$

$$\frac{1}{\tau_m^{ems}}\propto N_{\omega_0}+1$$

ODP scattering: Summary

$$\frac{1}{\tau_m(E)} = \frac{\pi D_O^2}{\rho \omega_0}\left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)\frac{D_{3D}(E \pm \hbar\omega_0)}{2}$$

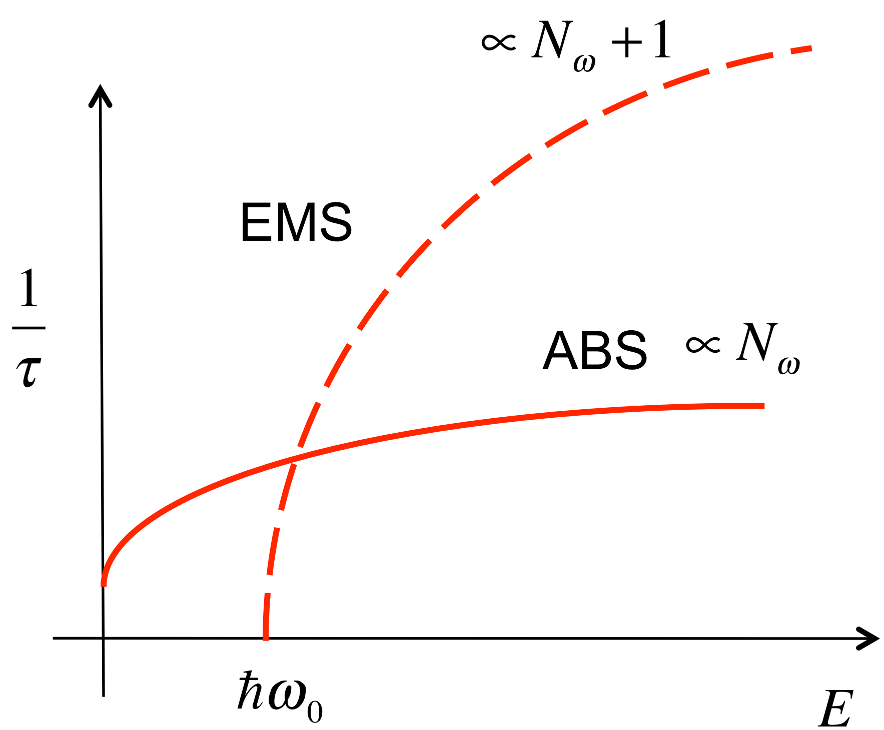


Power law scattering?

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

Absorption vs. emission

$$\frac{1}{\tau_m} = \frac{\pi D_O^2}{\rho \omega_0}\left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)\frac{D_{3D}(E)}{2}$$



Compare N and N+1 for GaAs at 300K:

$$\hbar\omega_0 = 0.033\,\mathrm{eV}$$

$$N_{\omega_0} = \frac{1}{e^{0.033/0.026} - 1} = 0.4$$

$$N_{\omega_0} + 1 = 1.4$$

Questions?

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