ECE-656: Fall 2009

Lecture 23: Phonon Scattering I

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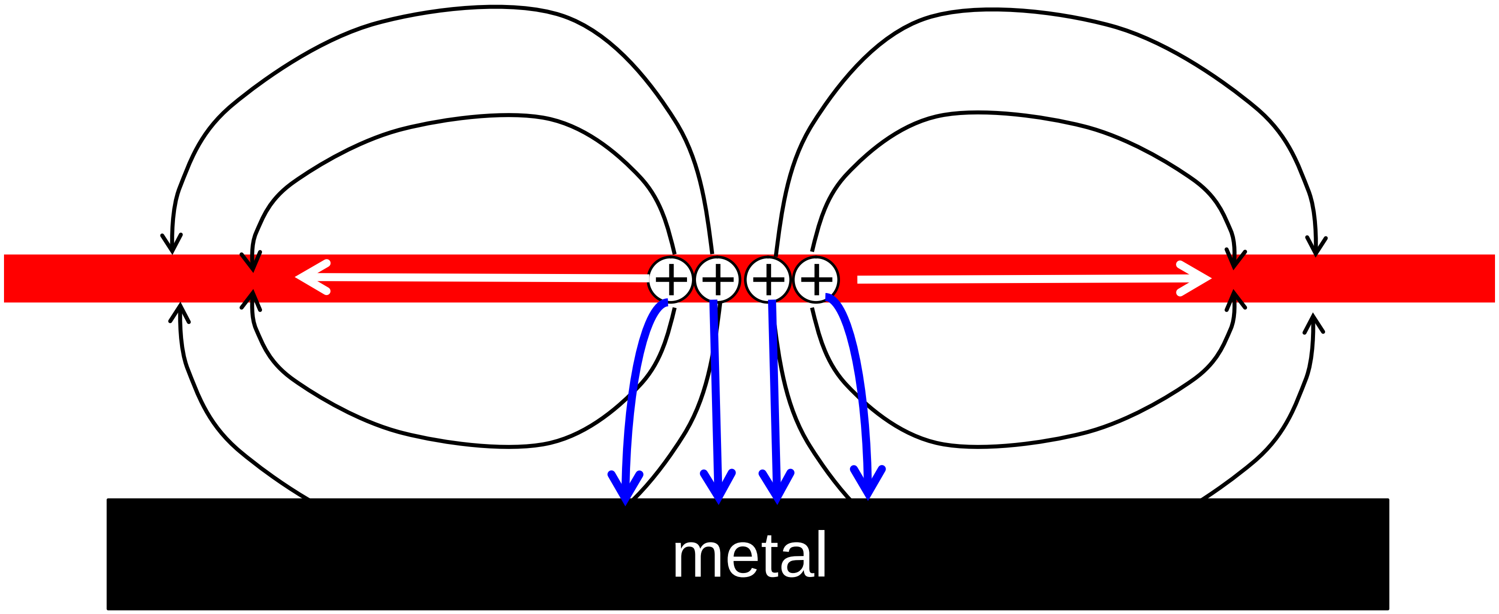
screening in 2D / 1D



geometric screening

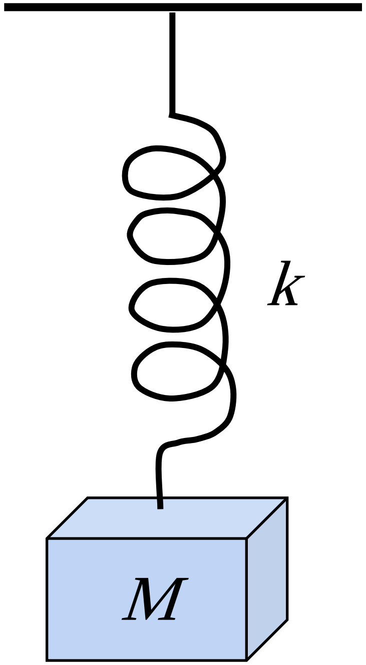
outline

1) **About phonons**

2) Electron-phonon coupling

3) Summary

springs



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

$$U = \frac{1}{2}k\left(x - x_0\right)^2$$

$$F = -\frac{dU}{dx} = -k\left(x - x_0\right)$$

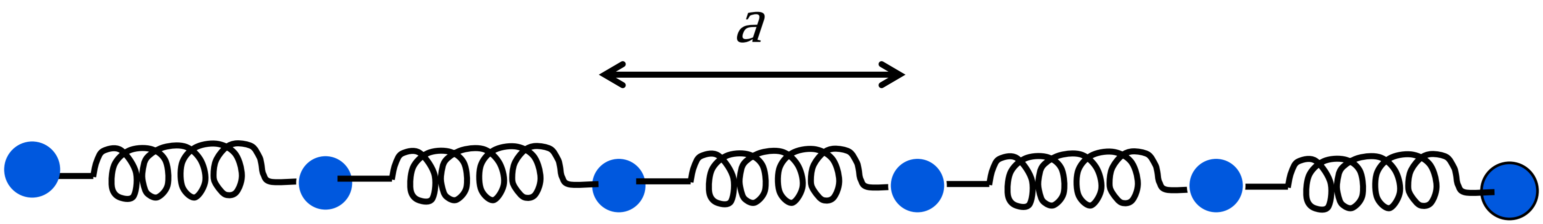
$$M\frac{d^2x}{dt^2} = -k\left(x - x_0\right)$$

$$x(t) - x_0 = Ae^{i\omega t}$$

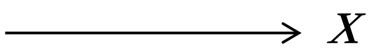
$$\omega = \sqrt{k/M}$$

$$E \sim A^2$$

lattice vibrations



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



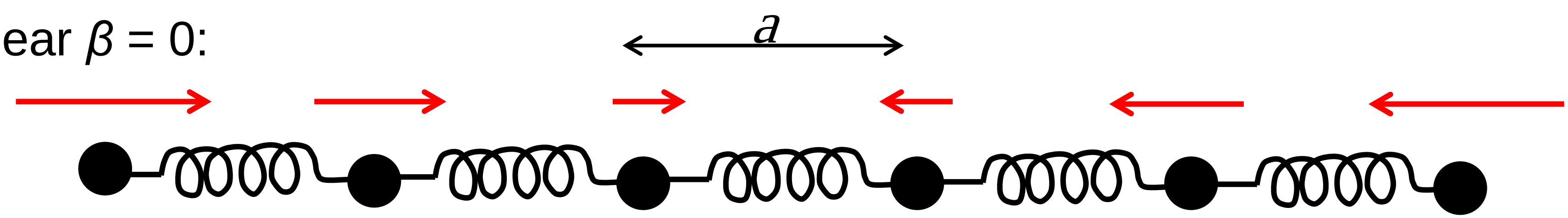
$\hat{e}_\nu = \hat{x}$ longitudinal

$\hat{e}_\nu = \hat{y}$ transverse

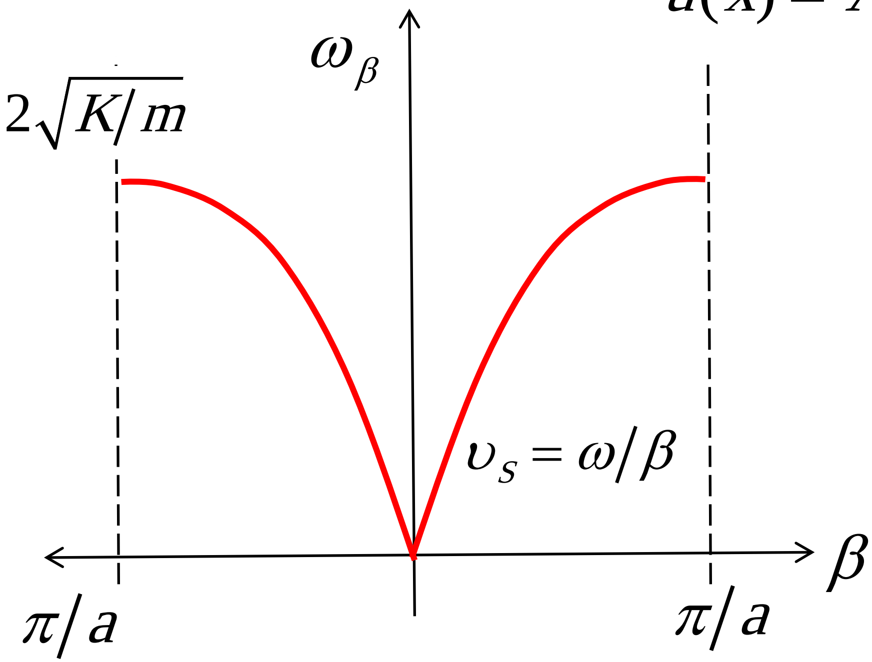
$\hat{e}_\nu = \hat{z}$ transverse

LA phonons (1)

near β = 0:



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



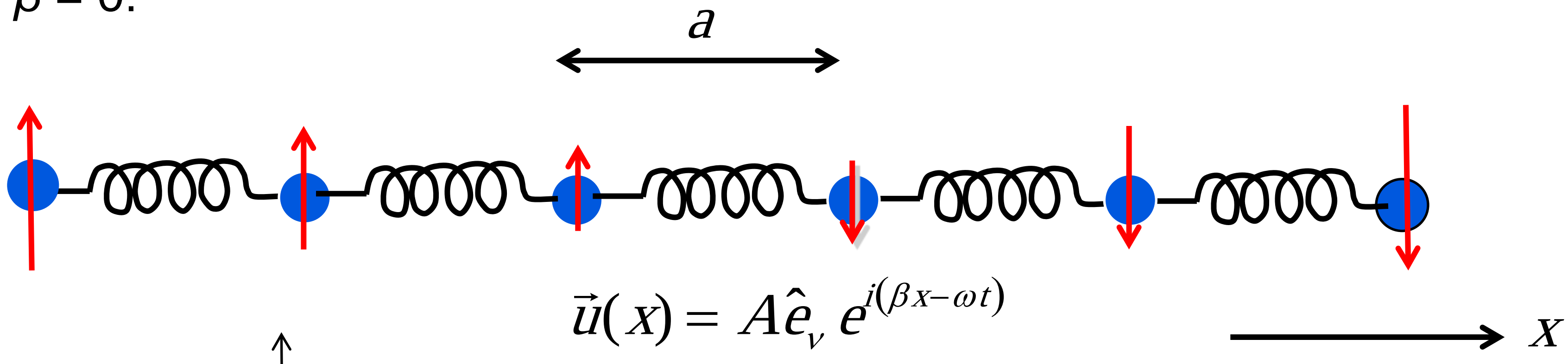
$$\omega(\beta) = 2\sqrt{\frac{K}{m}}\left|\sin\frac{\beta a}{2}\right| \quad \text{dispersion}$$

$$\upsilon_S = a\sqrt{K/m}$$

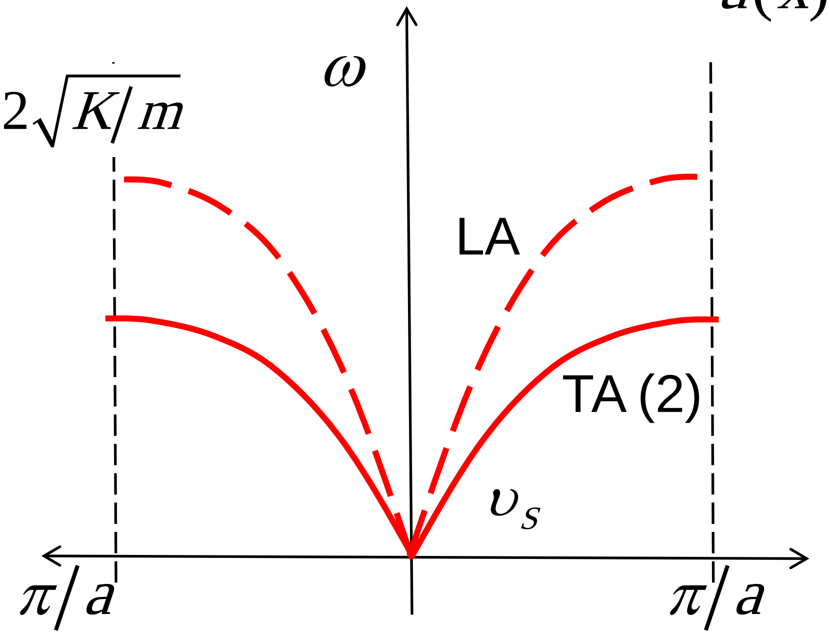
$$\omega/\beta = \upsilon_S = \sqrt{c_l/\rho} \approx 8.4\times 10^5 \text{ cm/s}$$

TA phonons (2)

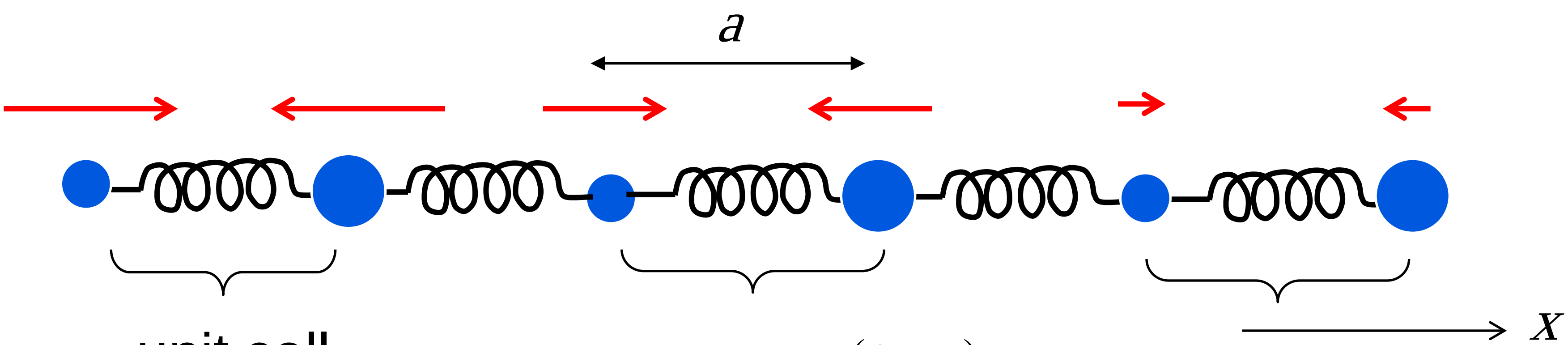
near $\beta = 0$:



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



LO phonons (1)

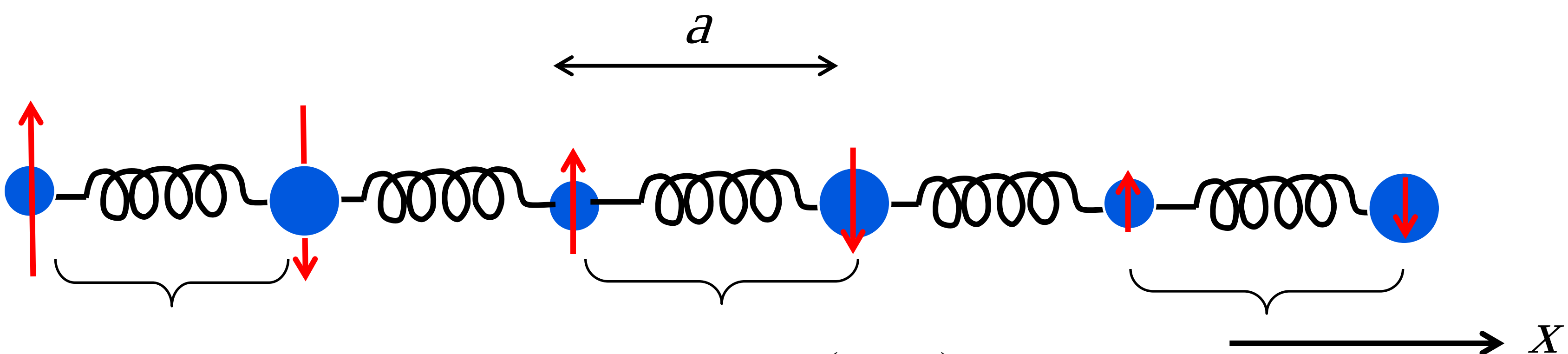


unit cell

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

the two atoms in a unit cell oscillate out of phase

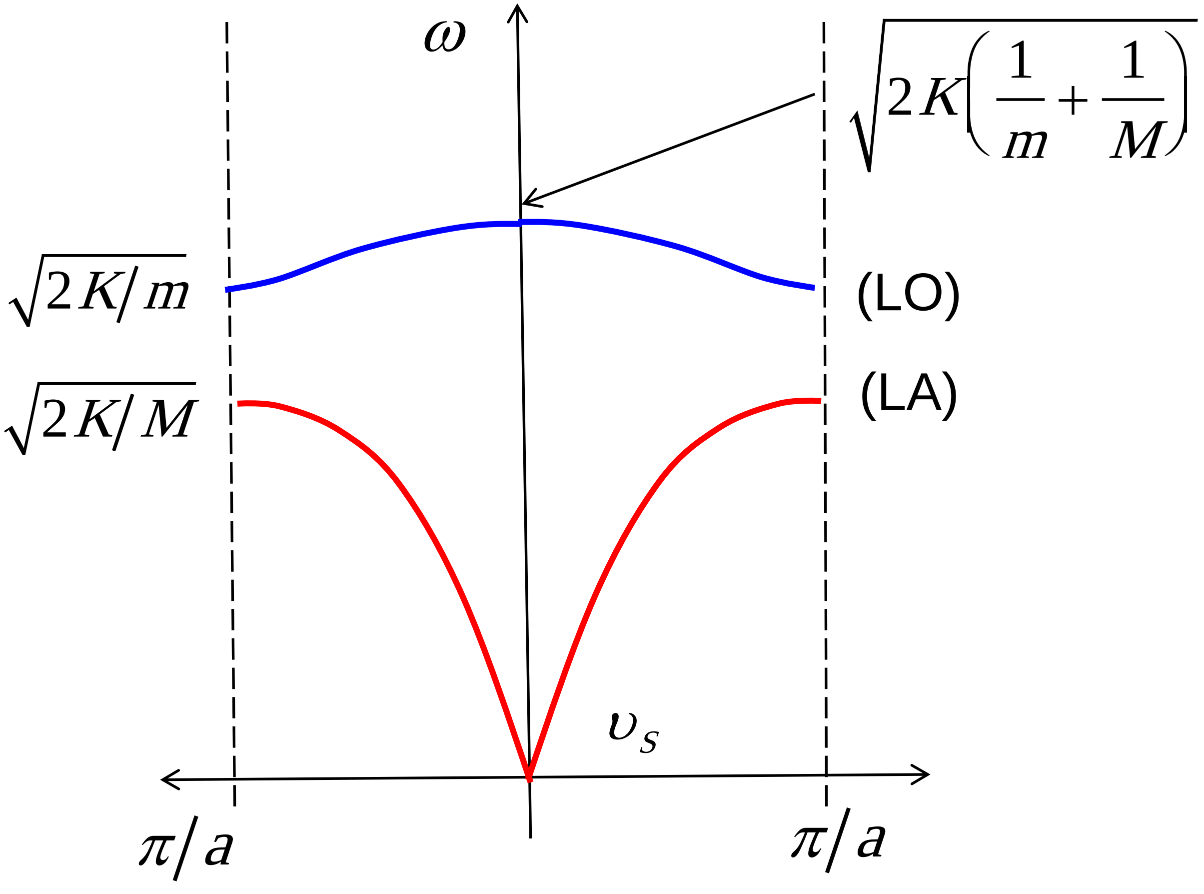
TO phonons (2)



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

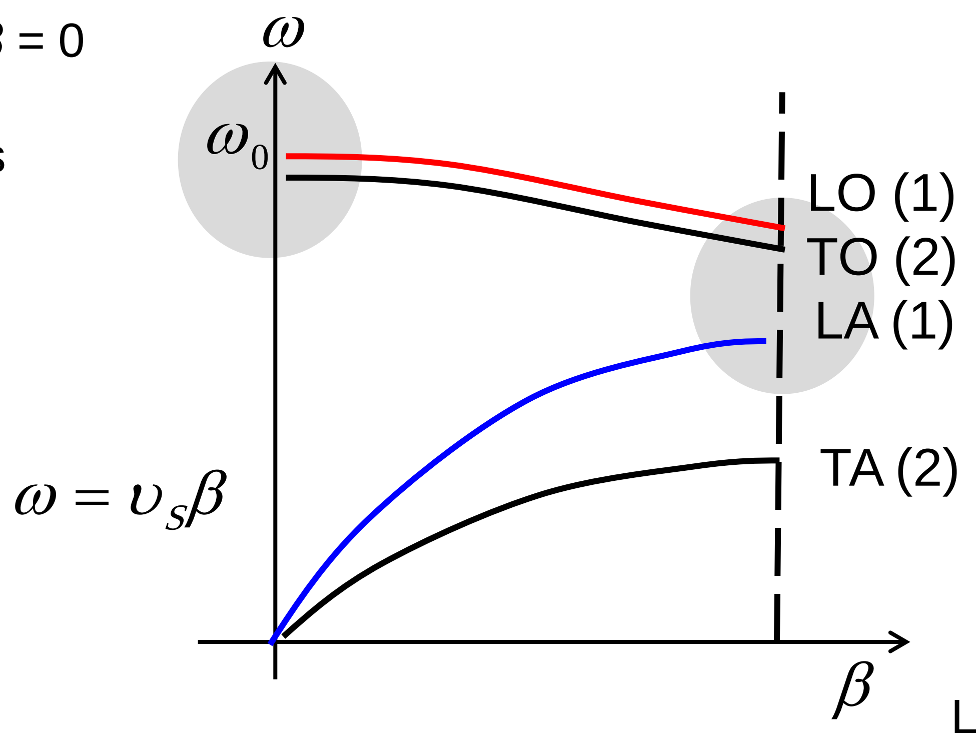
the two atoms in a unit cell oscillate out of phase

1D spring model (longitudinal modes)



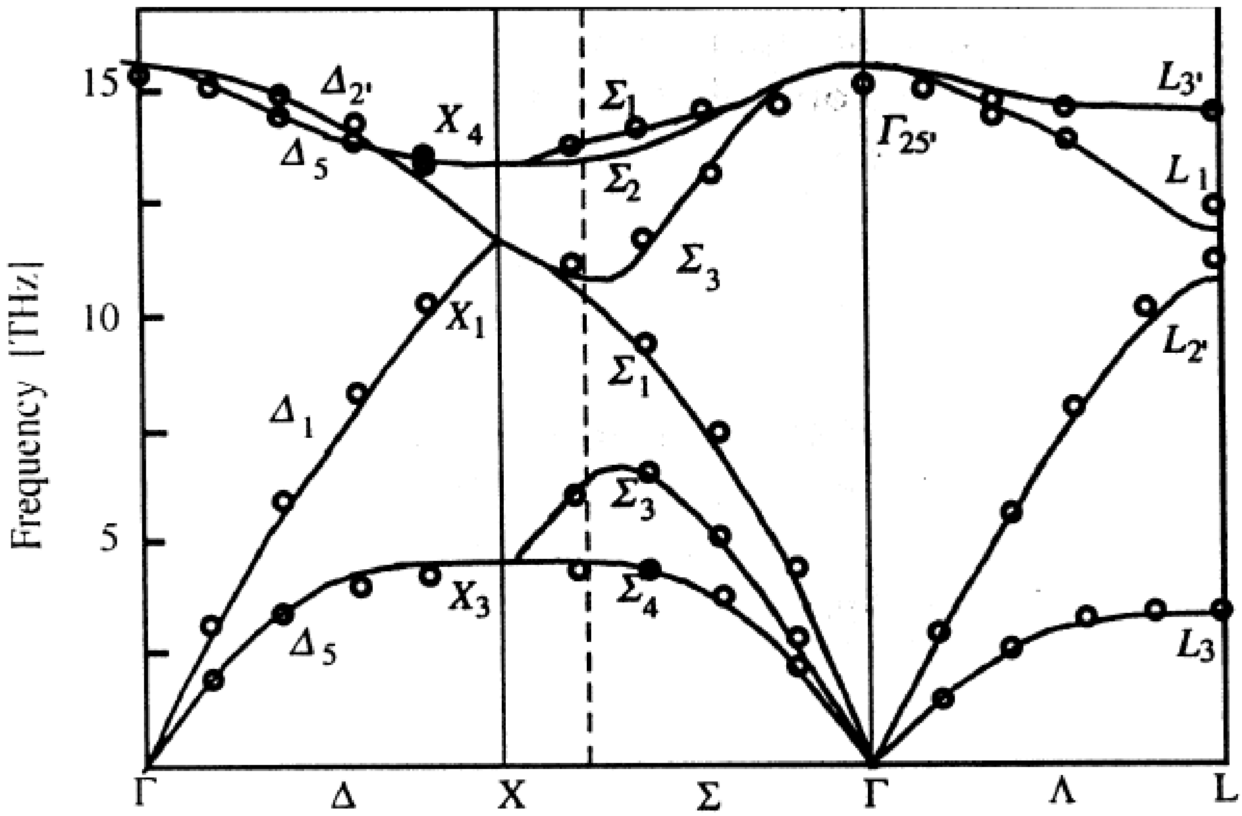
phonon dispersion characteristics

LO and TO degenerate at $\beta = 0$ for non polar semiconductors



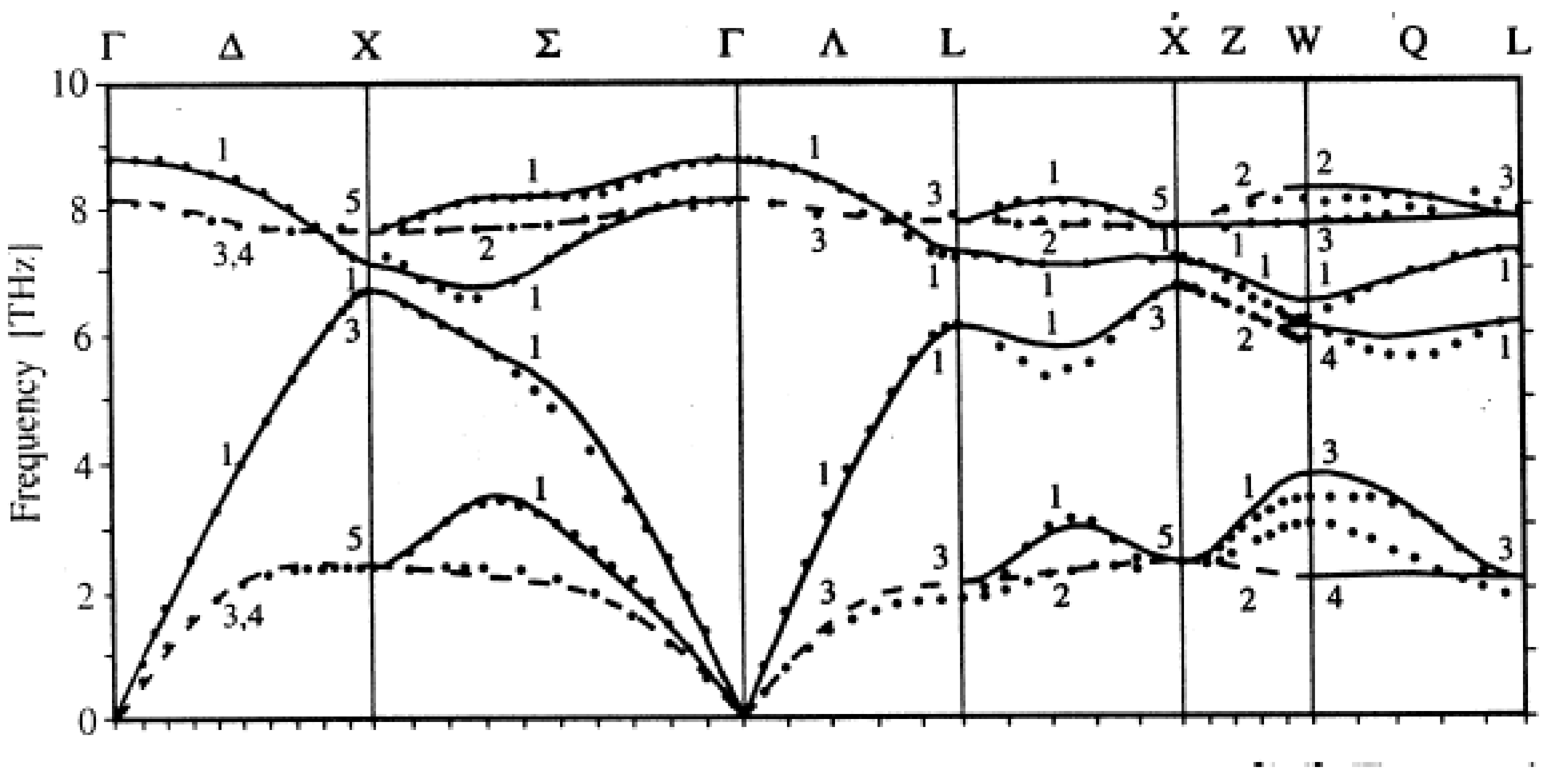
LO and LA degenerate at zone boundary for non polar semiconductors

measured phonon dispersion: Si



http://www.personal.psu.edu/pce3/Research%20Topics.htm

measured phonon dispersion: GaAs



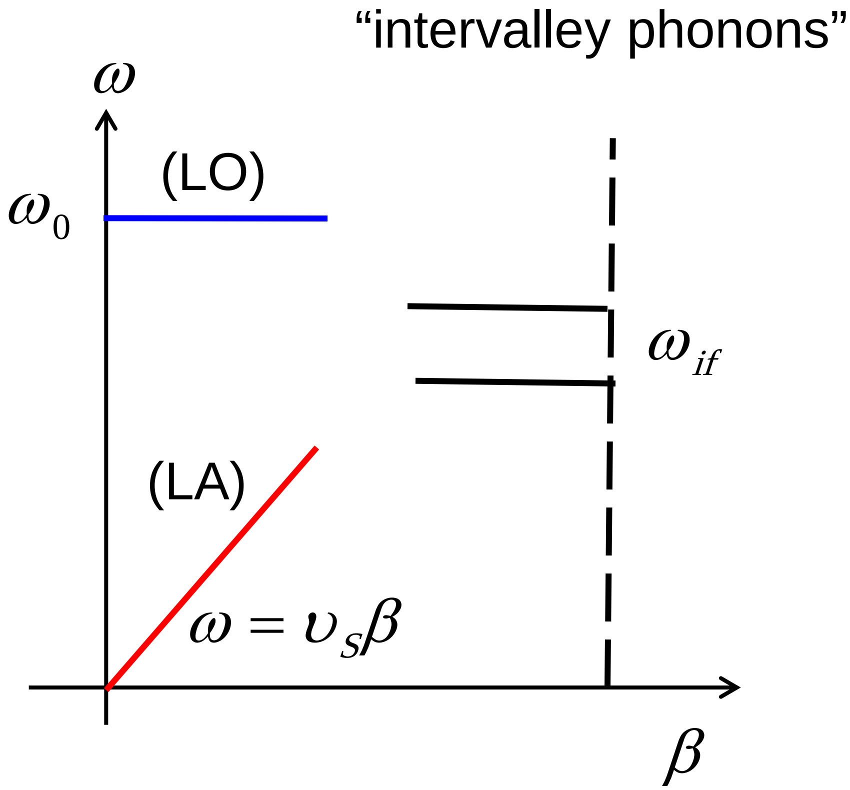
http://www.personal.psu.edu/pce3/Research%20Topics.htm

simplified phonon dispersion

1) Longitudinal modes couple most strongly with electrons.

2) Intravalley scattering requires small β.

3) Intervalley requires β near the Brillouin zone boundary.



amplitude of vibration

$$\vec{u}(x) = A\,\hat{e}_\nu \left[e^{i(\beta x - \omega t)} + e^{-i(\beta x - \omega t)} \right]$$

$$u(x_j) = 2|A|\cos\left(\beta a j - \omega_\beta t\right) \qquad x_j = a\,j$$

$$\frac{du_j}{dt} = 2|A|\,\omega \sin\left(\beta a j - \omega_\beta t\right)$$

$$\langle KE \rangle = \frac{1}{2} m \left\langle \left| \frac{du_j}{dt} \right|^2 \right\rangle = 2m|A|^2 \omega^2 \left\langle \sin^2\left(\beta a j - \omega_\beta t\right) \right\rangle = m|A|^2 \omega^2$$

$$\langle E \rangle = \langle KE \rangle + \langle PE \rangle = 2m|A|^2 \omega^2$$

$$\langle E_{TOT} \rangle = N_a 2m|A|^2 \omega^2 = \Omega \rho 2|A|^2 \omega^2$$

amplitude of vibration (ii)

$$\langle E_{TOT} \rangle = \Omega \rho 2 |A|^2 \omega^2$$

quantum mechanics says: $\langle E_{TOT} \rangle = \hbar\omega$

$$|A|^2 = \frac{\hbar}{2\Omega\rho\omega}$$

$$u_j = \left(A e^{i(\beta x - \omega t)} + cc\right) = 2|A|\cos\left(\beta a j - \omega_\beta t\right)$$

$$u_j = \sqrt{\frac{\hbar}{2\Omega\rho\omega}} \cos\left(\beta a j - \omega_\beta t\right)$$

$x = aj \quad j = 1, 2, 3, \ldots$

outline

1) About phonons

2) Electron-phonon coupling

3) Summary

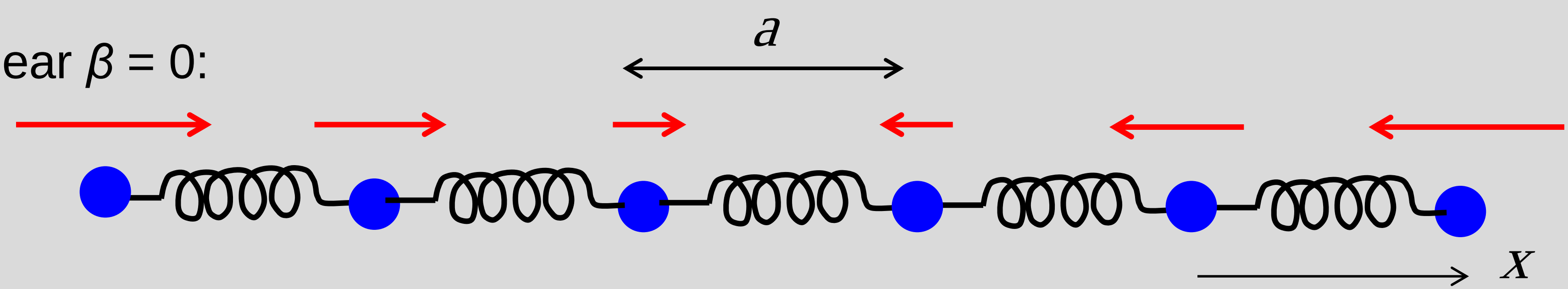
electron-phonon coupling (LA)

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'

LA phonons:

near $\beta = 0$:



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

$\dfrac{\delta a}{a} = \dfrac{\partial u}{\partial x}$ "strain"

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

deformation potential scattering

$$\frac{\delta a}{a} \approx \frac{\partial u}{\partial x}$$ "strain" $$U_S = \delta E_C = D_C \frac{\delta a}{a} = D_C \frac{\partial u_\beta}{\partial x}$$

$$u_\beta(x,t) = A_\beta e^{\pm i(\beta z - \omega t)}$$

$$U_S = D_A \frac{\partial u_\beta}{\partial x} = \pm i\beta D_A u_\beta = K_\beta u_\beta$$

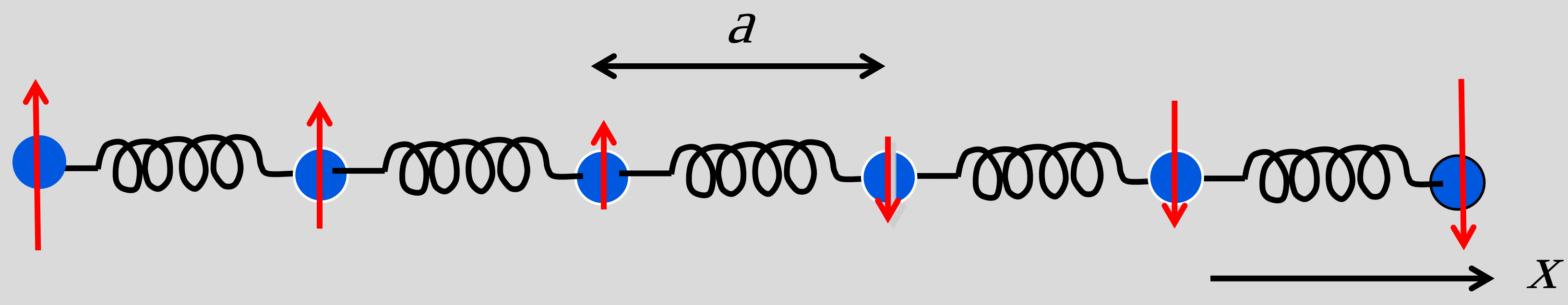
$$\left|K_\beta\right|^2 = \beta^2 D_A^2$$

"acoustic deformation potential scattering (ADP)"

electron-phonon coupling (TA)

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

near β = 0:

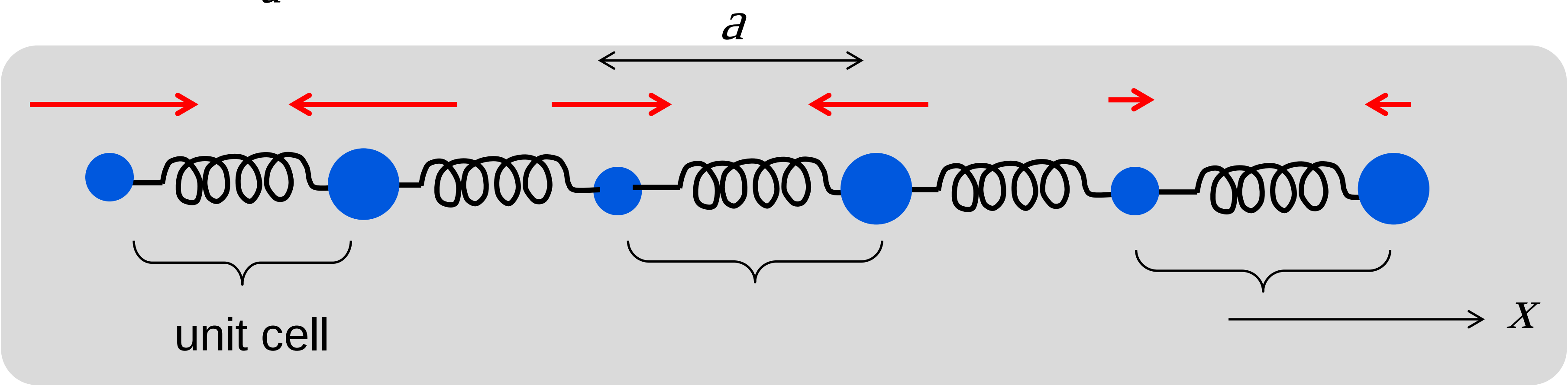


$$\frac{\delta a}{a} \propto \left(\frac{\partial u}{\partial x}\right)^2$$

To first order, *only* LA phonons scatter electrons

electron-phonon coupling (LO)

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

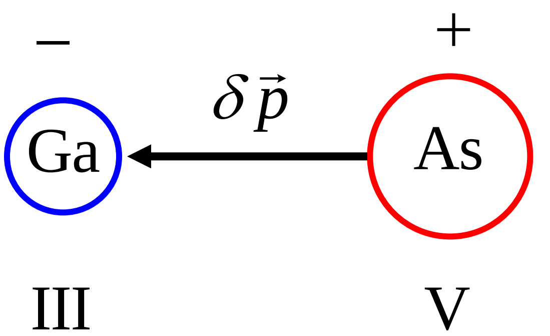


$$\delta a(x) = u_\beta(x) \qquad u_\beta(x,t) = A_\beta e^{\pm i(\beta z - \omega t)} \qquad U_S \approx D_O u_\beta = K_\beta u_\beta$$

$$\left|K_\beta\right|^2 = D_O^2$$

"optical deformation potential scattering (ODP)"

polar semiconductors



$$u_\beta(x,t) = A_\beta e^{\pm i(\beta z - \omega t)}$$

$$U_S = q\int \frac{\delta p_x}{\varepsilon_0 V_u}\,dx$$

$$\delta\vec{P} = \frac{\delta\vec{p}}{V_u}$$

$$D_x = \varepsilon_0 \mathcal{E}_x + P_x$$

$$\delta D = \varepsilon_0 \delta\mathcal{E} + \delta P$$

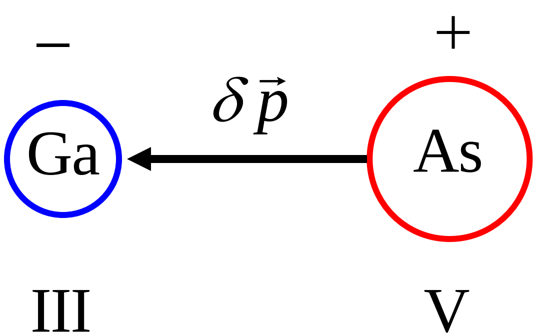
$$\nabla \bullet \delta D = 0$$

$$\delta D = \delta D_x e^{i\beta_x x} \rightarrow \delta D = 0$$

$$\delta\mathcal{E}_x = -\frac{\delta P_x}{\varepsilon_0} = -\frac{\delta p_x}{\varepsilon_0 V_u}$$

$$U_S = -q\int \mathcal{E}_x\,dx$$

optical phonons in polar semiconductors



$$u_\beta(x,t) = A_\beta e^{\pm i(\beta x - \omega t)}$$

$$\delta p = q^* u_\beta$$

$$U_S = \frac{q q^* u_\beta}{i\beta \varepsilon_0 V_u}$$

$$\left(\frac{q^*}{V_u}\right)^2 = \frac{\varepsilon_0 \rho \omega_0^2}{\kappa_0}\left(\frac{\kappa_0}{\kappa_\infty} - 1\right)$$

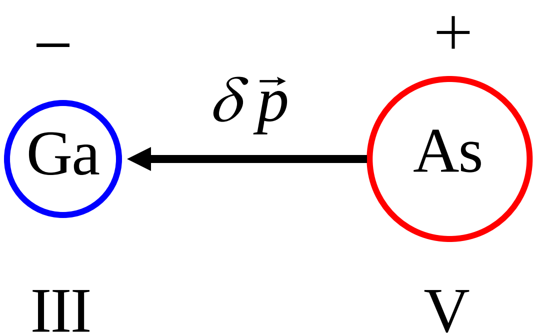
$$U_S = K_\beta u_\beta$$

$$U_S = q\int \frac{\delta p_x}{\varepsilon_0 V_u} dx$$

$$\left|K_\beta\right|^2 = \frac{\rho q^2 \omega_0^2}{\beta^2 \kappa_0 \varepsilon_0}\left(\frac{\kappa_0}{\kappa_\infty} - 1\right)$$

small angle scattering dominates

acoustic phonons in polar semiconductors



$$\delta p = q^* \frac{\partial u_\beta}{\partial x} = q^* i \beta u_\beta$$

$$U_S = \frac{q q^*}{\varepsilon_0 V_u} u_\beta = \frac{q e_{PZ}}{\kappa_0 \varepsilon_0} u_\beta$$

$$U_S = K_\beta u_\beta$$

$$u_\beta(x,t) = A_\beta e^{\pm i(\beta x - \omega t)}$$

$$U_S = q \int \frac{\delta p_x}{\varepsilon_0 V_u} dx$$

$$\left| K_\beta \right|^2 = \frac{q^2 e_{PZ}^2}{\kappa_0^2 \varepsilon_0^2}$$

scattering potentials

$$u_\beta(\vec{r},t) = A_\beta e^{\pm i\left(\vec{\beta}\bullet\vec{r} - \omega_\beta t\right)} \qquad U_S = K_\beta u_\beta$$

ADP $\quad |K_\beta|^2 = \beta^2 D_A^2$

ODP $\quad |K_\beta|^2 = D_O^2$

PZ $\quad |K_\beta|^2 = \left(q e_{PZ}/\kappa_S \varepsilon_0\right)^2$

POP $\quad |K_\beta|^2 = \dfrac{\rho q^2 \omega_0^2}{\beta^2 \kappa_0 \varepsilon_0}\left(\dfrac{\kappa_0}{\kappa_\infty} - 1\right)$

other scattering mechanisms

1) Neutral impurity

2) Alloy scattering

3) Surface / edge roughness scattering

4) Plasmon scattering

5) Electron-electron scattering

6) Electron-hole

questions

1) About phonons

2) Electron-phonon coupling

3) Summary