Lecture contents

- Coupled oscillators
- Dispersion relationship
- Acoustical and optical lattice vibrations
- Acoustical and optical phonons
- Phonon statistics
- Acoustical phonon scattering

Few concepts from Solid State Physics
1. Adiabatic approximation

When valence and core ectrons are separated, general Schrödinger equation for a condensed medium without spin

$$H = \sum_l \frac{\mathbf{p}_l^2}{2M_l} + \sum_{l,m} U(\mathbf{R}_l - \mathbf{R}_m) + \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i,l} V(\mathbf{r}_i - \mathbf{R}_l) + \sum_{i,j} \frac{e^2/4\pi\epsilon_0}{|\mathbf{r}_i - \mathbf{r}_j|} = H_L + H_e$$

$$H\Psi(R,r) = E\Psi(R,r)$$

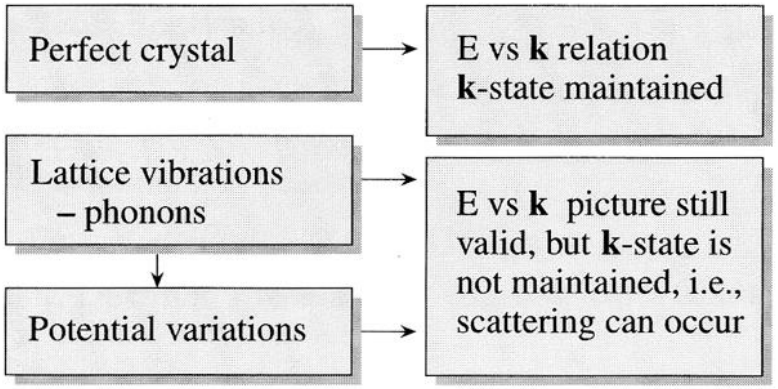
- Mass of ions >1000 (for most semiconductors >10^2 times greater than mass of electrons
- Ion velocities >100 times slower
- Electrons adjust 'instantaneously" to the positions of atoms

$$\Psi(R,r) \approx \psi(r,R_0)\Phi(R)$$

$$\Rightarrow \quad H_L\Phi(R) = E_L\Phi(R)$$

$$H_e\psi(r,R) = E_e\psi(r,R)$$

- Separate ion and electron motion (accuracy ~m/M)



Few concepts from Solid State Physics
2. Phonons

Hamiltonian for lattice motion (harmonic oscillations) :

$$H_L = \sum_l \frac{p_l^2}{2M_l} + \sum_{l,m} U_0\left(R_l^0 - R_m^0\right) + \sum_{l,m} \frac{1}{2} C_{l,m}\left(u_l - u_m\right)^2 + U_{anhar}$$

Displacements show up as plane waves with weak interaction via anharmonicity:

$$u_{k,\omega} = u_0 e^{ikr - i\omega t}$$

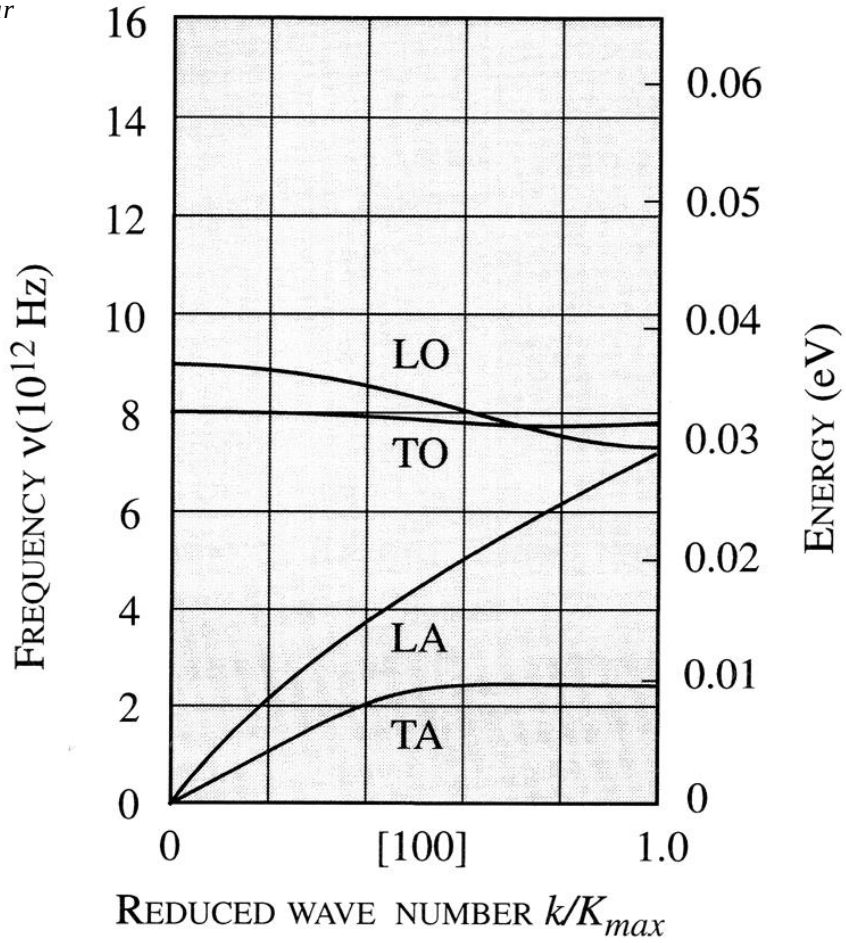
Energy in a mode:

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

Equilibrium distribution (Bose Einstein):

$$n(\omega) = \frac{1}{\exp\left(\frac{\hbar\omega}{kT}\right) - 1}$$

Phonon dispersion relation in GaAs

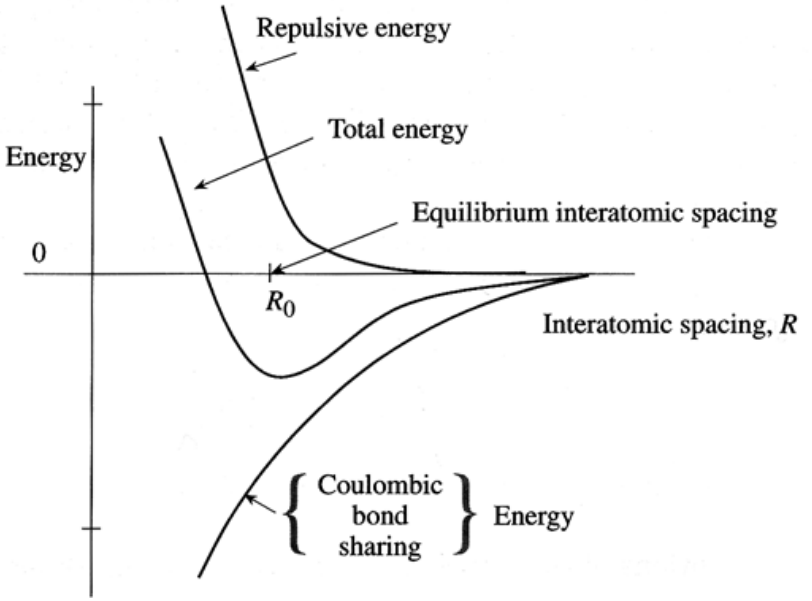


Lattice vibrations

Lattice Hamiltonian:

$$H_L = \sum_l \frac{p_l^2}{2M_l} + \sum_{l,m} U\left(R_l^0 - R_m^0\right)$$

Binding energy vs. interatomic distance in a crystal



Expanding binding energy around the equilibrium position R_0:

$$U(R) = U(R_0) + \left(\frac{dU}{dR}\right)_{R_0} \Delta R + \frac{1}{2}\left(\frac{d^2U}{dR^2}\right)_{R_0} \Delta R^2 + \ldots$$

$\left(\frac{dU}{dR}\right)_{R_0} \to 0$

Linear term is zero at minimum

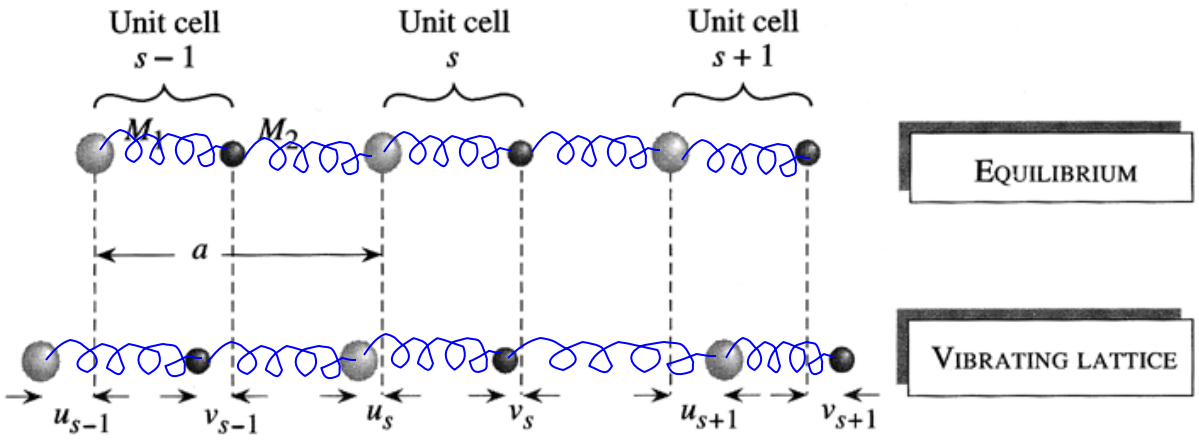
Neglecting anharmonic terms:

$$U(R) = U(R_0) + \frac{1}{2} C\left(\Delta R\right)^2$$

with a force constant C

Diatomic chain

Let's consider diatomic chain to demonstrate acoustical and optical dispersion branches



Masses are connected by springs w equal spring constants, *C*, for simplicity

Force = - C ·ΔR

With *u* and *v*, the displacements of respective atoms, we can write down classical equation of motion (second Newton law)

$$\begin{cases} M_1 \dfrac{d^2 u_s}{dt^2} = C\left(v_s + v_{s-1} - 2u_s\right) \\ M_2 \dfrac{d^2 v_s}{dt^2} = C\left(u_{s+1} + u_s - 2v_s\right) \end{cases}$$

The solution for displacements in the chain will be searched as traveling waves:

$$\begin{cases} u_s = u e^{iksa - i\omega t} \\ v_s = v e^{iksa - i\omega t} \end{cases}$$

From Singh, 2003

Solution for diatomic chain

$$\begin{cases} M_1(-\omega^2)u\,e^{ikxa-i\omega t} = C\left(v + ve^{-ika} - 2u\right)e^{ikxa-i\omega t} \\ M_2(-\omega^2)v = C\left(ue^{ika} + u - 2v\right) \end{cases}$$

$$\begin{cases} u\left(-\omega^2 M_1 + 2C\right) - vC\left(1+e^{-ika}\right) = 0 \\ -uC\left(1+e^{ika}\right) + v\left(-\omega^2 M_2 + 2C\right) = 0 \end{cases}$$

For nontrivial solutions, determinant should be zero

$$\left(2C-\omega^2 M_1\right)\left(2C-\omega^2 M_2\right) - C^2\left(1+e^{-ika}\right)\left(1+e^{ika}\right) = 0$$

$$M_1M_2\omega^4 - 2C(M_1+M_2)\omega^2 + 4C^2 - C^2\underbrace{\left[1+e^{-ika}+e^{ika}+1\right]}_{2+2\cos ka} = 0$$

$$M_1M_2\omega^4 - 2C(M_1+M_2)\omega^2 + 2C^2(1-\cos ka) = 0$$

$$\omega^2 = \frac{2C(M_1+M_2) \pm \sqrt{4C^2(M_1+M_2)^2 - 8C^2M_1M_2(1-\cos ka)}}{2M_1M_2}$$

small k:

$$\cos ka \approx 1 - \frac{(ka)^2}{2}$$

$$\omega^2 = \frac{2C(M_1+M_2) \pm \sqrt{4C^2(M_1+M_2)^2 - 8C^2M_1M_2\frac{(ka)^2}{2}}}{2M_1M_2} =$$

$$\approx \frac{2C(M_1+M_2)}{2M_1M_2}\left[1 \pm \left(1 - \frac{1}{2}\frac{M_1M_2(ka)^2}{(M_1+M_2)^2}\right)\right]$$

acoustical: $(-)$

$$\omega_{ac}^2 = \frac{C(M_1+M_2)}{M_1M_2}\frac{M_1M_2}{(M_1+M_2)^2}\cdot\frac{1}{2}(ka)^2 = \frac{C}{2}\frac{k^2a^2}{M_1+M_2}$$

optical: $(+)$

$$\omega_{opt}^2 = \frac{C(M_1+M_2)}{M_1M_2}\left[\frac{4(M_1+M_2)^2 - M_1M_2(ka)^2}{2(M_1+M_2)^2}\right] \simeq \quad \text{(small)}$$

$$\simeq \frac{2C(M_1+M_2)}{M_1M_2} = 2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right)$$

$$K = \pm\frac{\pi}{a} \qquad \cos(\pm\pi) = -1$$

$$\omega^2 = \frac{2C(M_1+M_2) \pm \sqrt{4C^2\left(M_1^2+M_2^2+2M_1M_2-4M_1M_2\right)}}{2M_1M_2} =$$

$$\simeq \frac{2C(M_1+M_2) \pm 2C(M_1-M_2)}{2M_1M_2}$$

acoust: $(-)$

$$\omega_{ac}^2 = \frac{2C}{M_1}$$

optical: $(+)$

$$\omega_{opt}^2 = \frac{2C}{M_2}$$

Dispersion relations for diatomic chain

$$\omega^2 = \frac{2C(M_1+M_2) \pm \sqrt{4C^2(M_1+M_2)^2 - 8C^2M_1M_2(1-\cos ka)}}{2M_1M_2}$$

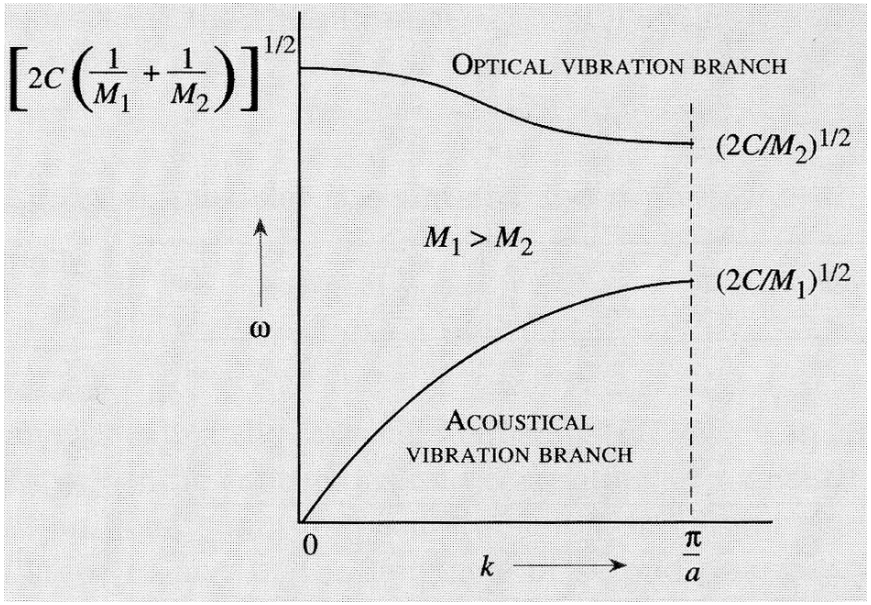
Solutions for small k : $\omega_{ac}^2 = \frac{C}{2}\frac{k^2a^2}{M_1+M_2}$

$$\omega_{opt}^2 = 2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right)$$

Solutions for the edge of Brillouin zone $k=\pi/a$:

$$\omega_{ac}^2 = \frac{2C}{M_1}$$

$$\omega_{opt}^2 = \frac{2C}{M_2}$$



From Singh, 2003

Acoustical and optical waves

For acoustical branch in long wavelength limit (at small k):

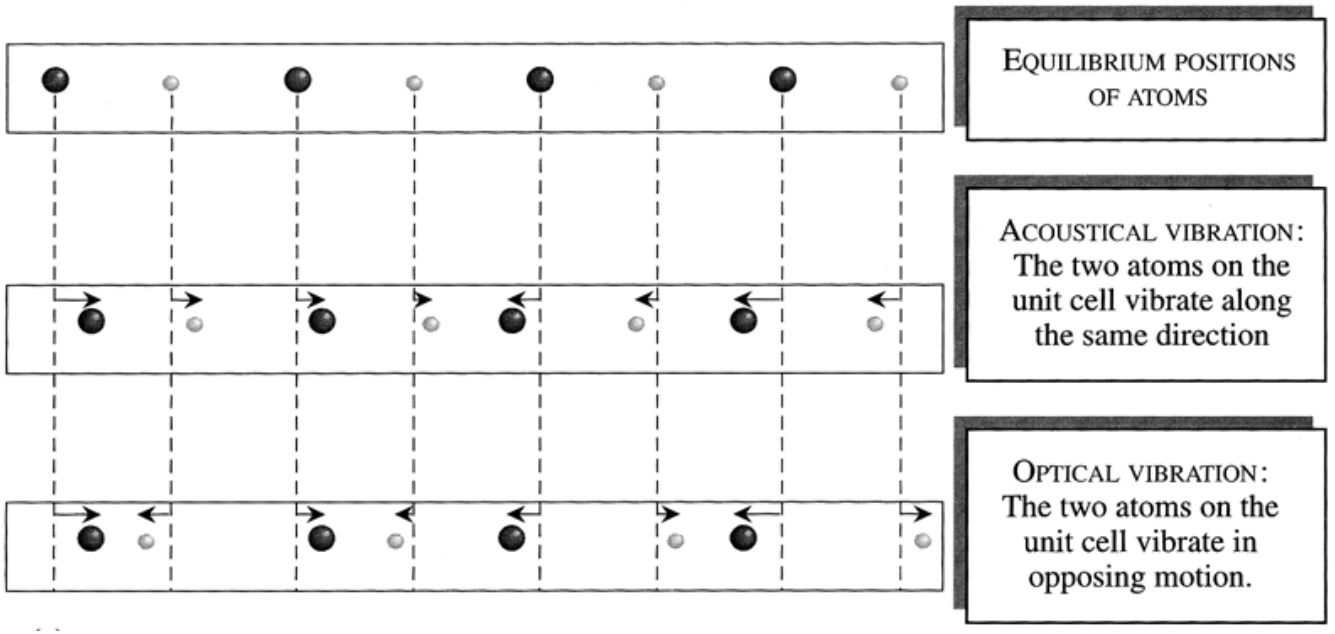
$$u \approx v \qquad or \qquad u_s \approx v_s$$

Sound velocity:

$$v_s = \frac{d\omega}{dk} = \frac{a}{2}\sqrt{\frac{C}{M_{av}}}$$

For optical branch at $k=0$:
(Two atoms vibrate against their center of masses)

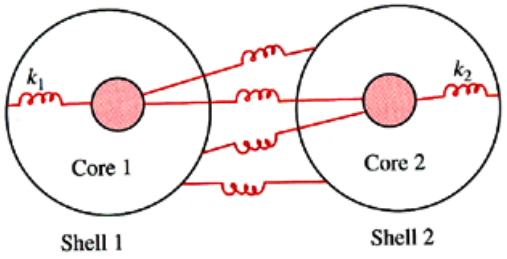
$$u \approx -\frac{M_2}{M_1} v$$



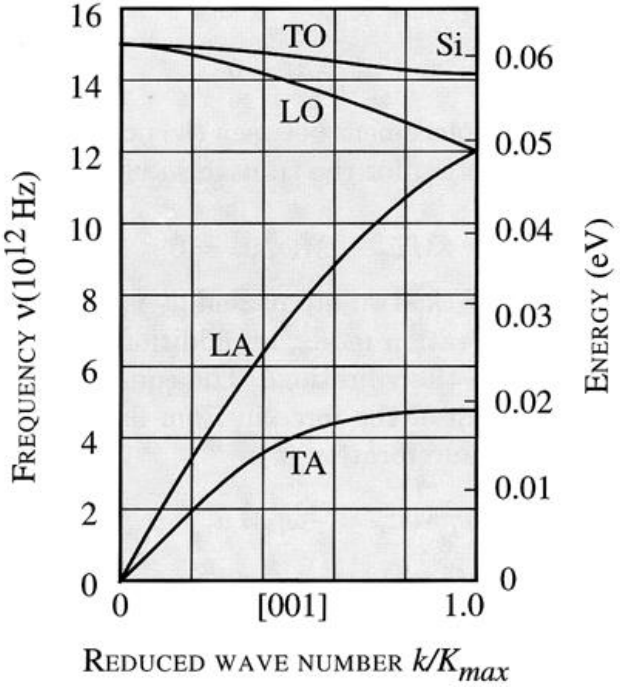
Dispersion curves in semiconductor crystals

- For each wavevector there are 1 longitudinal mode and 2 transverse modes
- The frequencies are determined by force constants
- Usually longitudinal mode (LA) is stiffer
- Energy scales (for similar crystals) as $M^{-1/2}$
- Atomic vibrations are in THz range

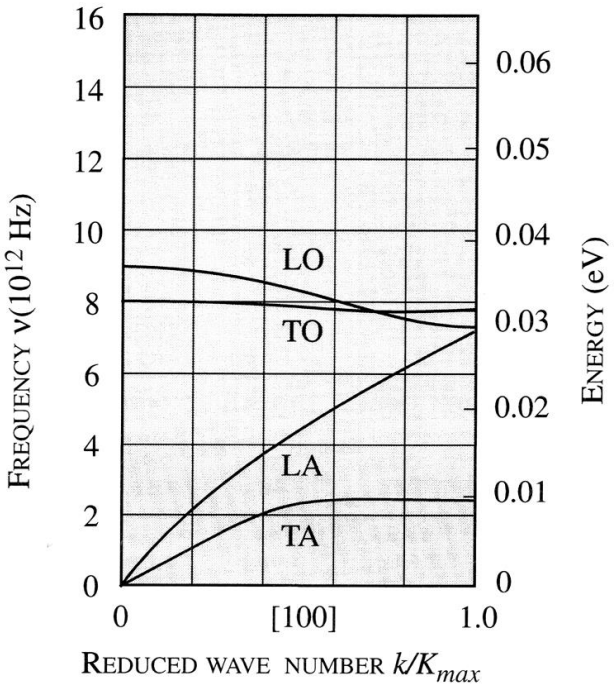
Example: shell model



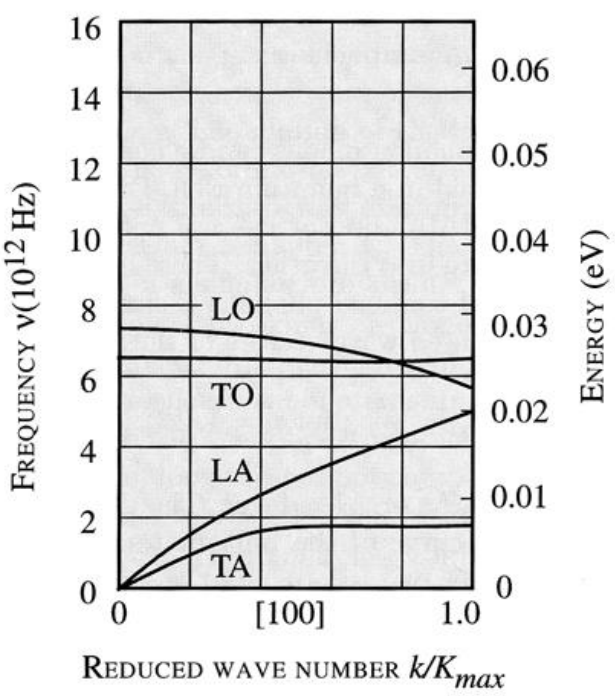
Si



GaAs



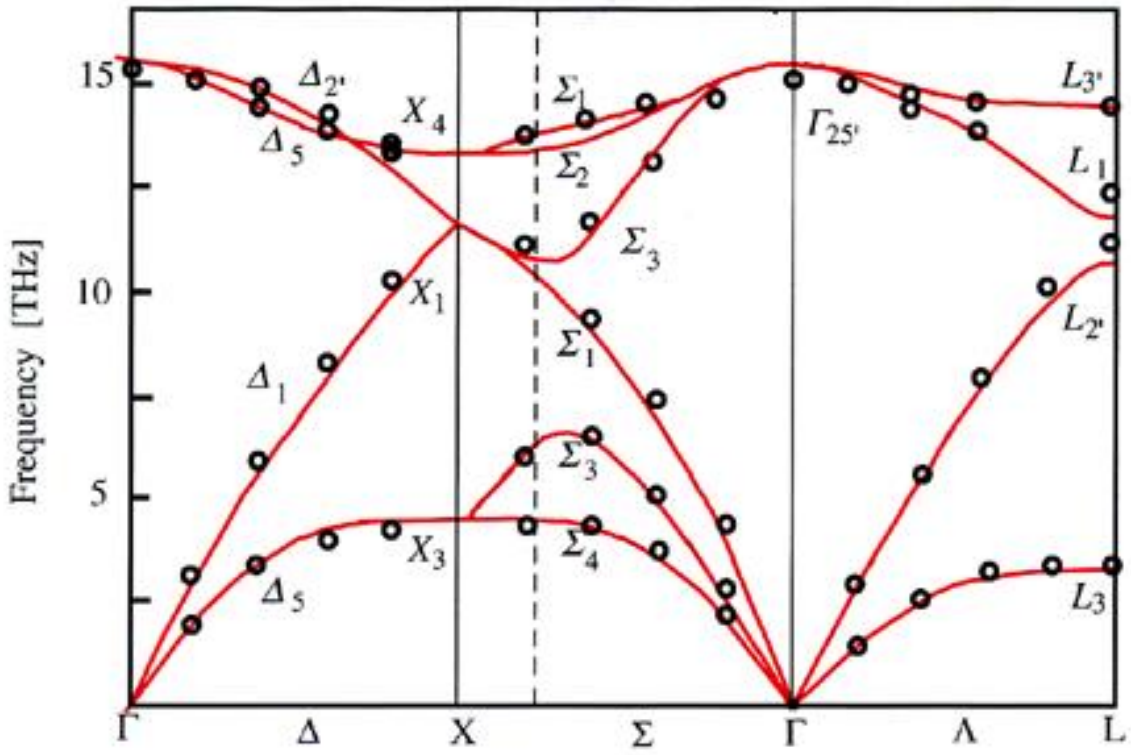
InAs



From Singh, 2003

Anisotropy of phonon dispersion curves

Experimental (points) and calculated phonon dispersion curves for Si

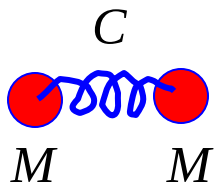


From Yu, Cordona, 2002

Quantum harmonic oscillator

Quantum harmonic oscillator: Hamiltonian

$$H = \frac{p^2}{2M} + \frac{1}{2}Cx^2$$

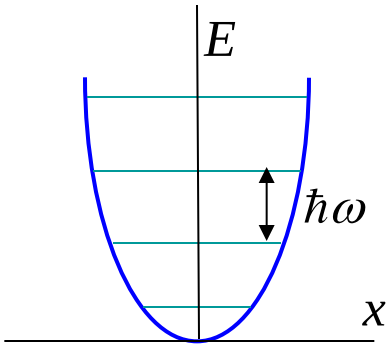


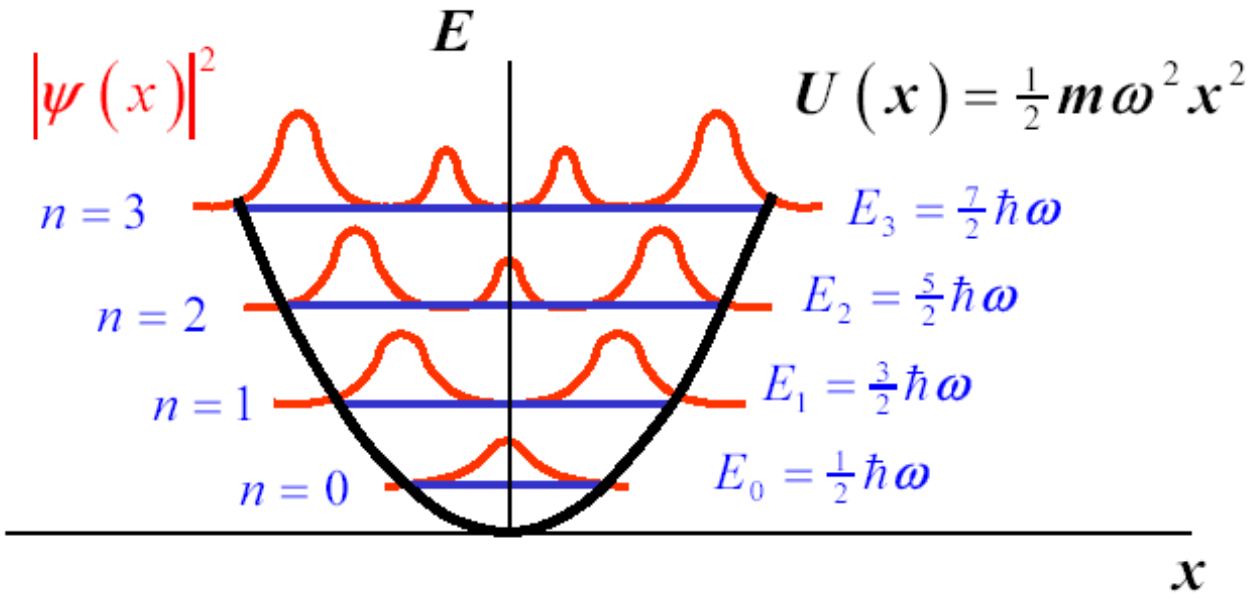
Solution gives resonance frequency (as in classical mechanics)

$$\omega^2 = \frac{C}{M}$$

And quantum oscillation spectrum:
(n may be considered as number of "quasiparticles")

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





Quantization of lattice vibrations: phonons

For a single oscillator the frequency is fixed, but when many oscillators interact we have a number of modes (normal modes)

$$\omega_k$$

Each mode is occupied by n_k phonons

$$E_k = \left(n_k + \frac{1}{2} \right) \hbar \omega_k$$

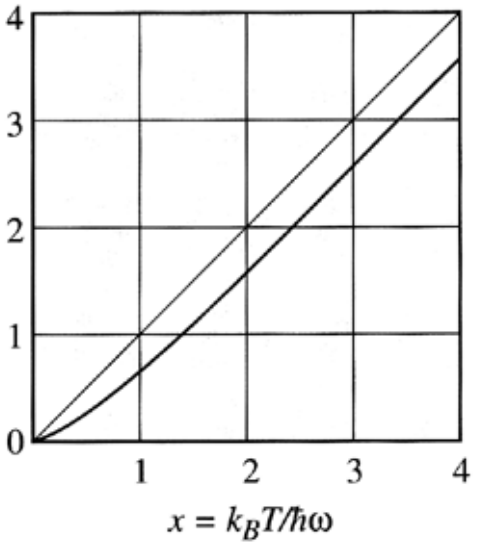
For a 1D chain states are determined as:

$$k = \frac{2\pi m}{Na}; \; for \quad n = 0, \pm 1, \ldots \pm \frac{N}{2}$$

Occupancy of modes is given by Bose-statistics:

$$n(\omega) = \frac{1}{\exp\left(\frac{\hbar \omega}{kT} \right) - 1}$$

Bose-Einstein distribution function



Optical phonons: Raman scattering

- Inelastic light scattering = Raman scattering gives information on optically active vibrations in a material
- Wavevector of photons is SMALL
- Stokes (creation of vibration) and anti-Stokes (emission of vibration)
- Symmetry and selection rules: Raman scattering intensity depends on geometry and polarization

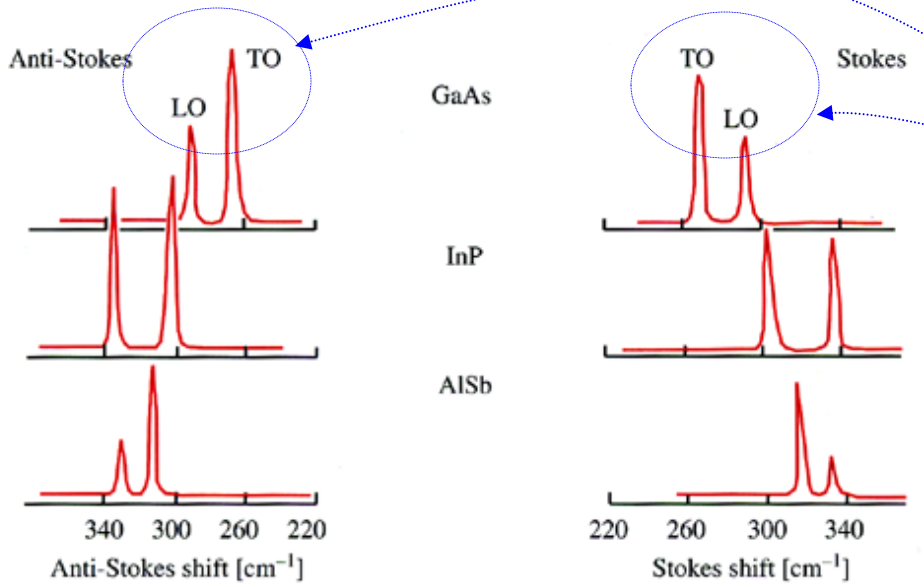
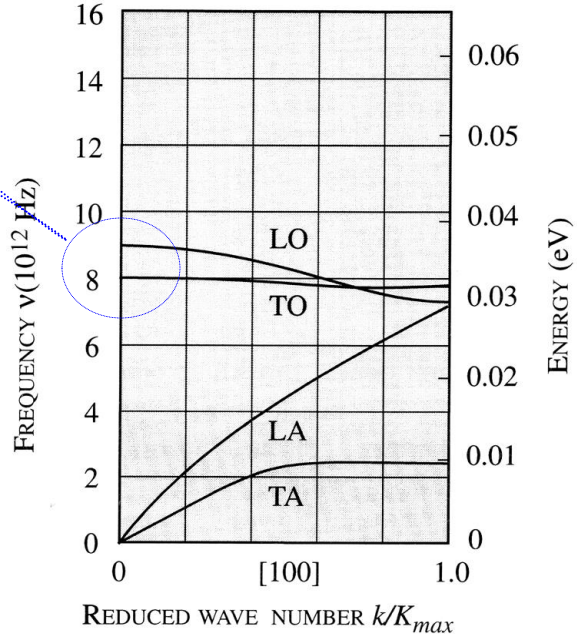


Fig. 7.21. Raman spectra of three zinc-blende-type semiconductors showing the TO and LO phonons in both Stokes and anti-Stokes scattering. Note that the vertical scales are not the same for all spectra.

GaAs



From Yu and Cordona, 2003

Lattice scattering rate calculation

Goal: calculation of the scattering integral or relaxation time:

$$\left.\frac{\partial f}{\partial t}\right|_{coll} = \frac{f - f_0}{\tau} = \int \left[f_{k'}(1 - f_k) W(k', k) - f_k (1 - f_{k'}) W(k, k') \right] \frac{d^3 k'}{(2\pi)^3}$$

Step 1. Determine scattering potential $H \propto e^{iqr - i\omega t}$

Step 2. Calculate matrix elements from *k'* to *k* $H_{k'k} = \int_V \psi_{k'}^* H \psi_k d^3 r$

Step 3. Calculate transition rate from *k'* to *k* using "golden Fermi rule" $W(k', k) = \frac{2\pi}{\hbar} \left| H_{k'k} \right|^2 \delta\left(E(k) - E(k') - \hbar\omega \right)$

Step 4. Calculate state relaxation time $\left.\frac{\partial f}{\partial t}\right|_{coll} = \frac{f - f^0}{\tau(k)} = \sum f_{k'}(1 - f_k) W(k', k) - f_k (1 - f_{k'}) W(k, k')$

Step 5. Average relaxation time $\langle \tau(k) \rangle$