Condensed Matter Physics I

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Previously

- Binding Attractive and repulsive potentials
- Lattice sums, cohesive energy, equilibrium structure

- Reciprocal space
- Diffraction

Today

- Phonons (Ch.4 & 5 Kittel)

PHONONS

Elementary excitations in solids

Charge	Electronic excitations
EM field	Photon
Elastic	Phonon
Magnetic	Magnon (spin-wave)
Multi-particle	Exciton, polariton, polaron
Collective	Plasmon
…	…

Phonons

- Propagation of sound
- Optical properties (infrared)
- Lattice expansion
- Heat capacity
- Thermal conductivity

General

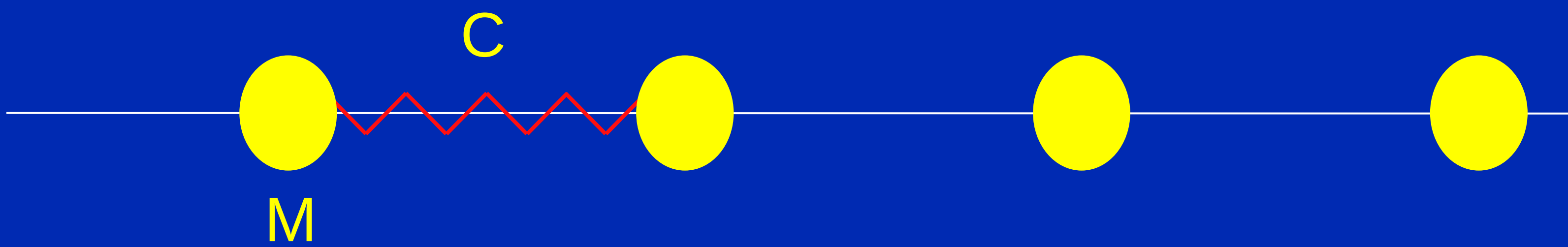
Total lattice energy $U_{total} = \sum_{<ij>} U_{ij}(\vec{R}_j - \vec{R}_i)$

Stability: $\Delta_{R_j} U_{total} = 0 \Rightarrow$ Equilibrium coordinates

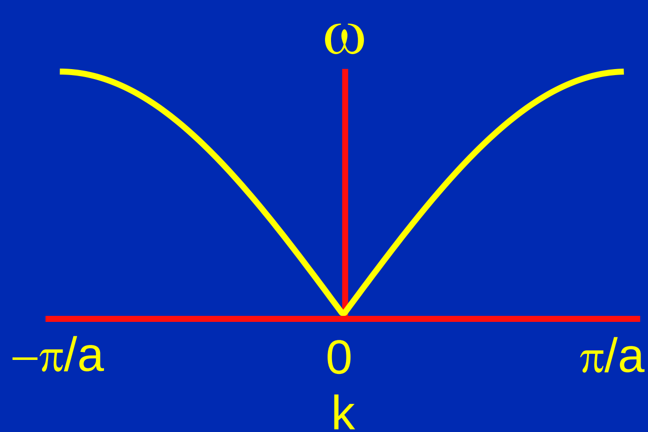
<u>Harmonic approximation:</u>

$$F_j = -\frac{\partial U_{total}}{\partial R_j}$$

1D, 1 at./cell

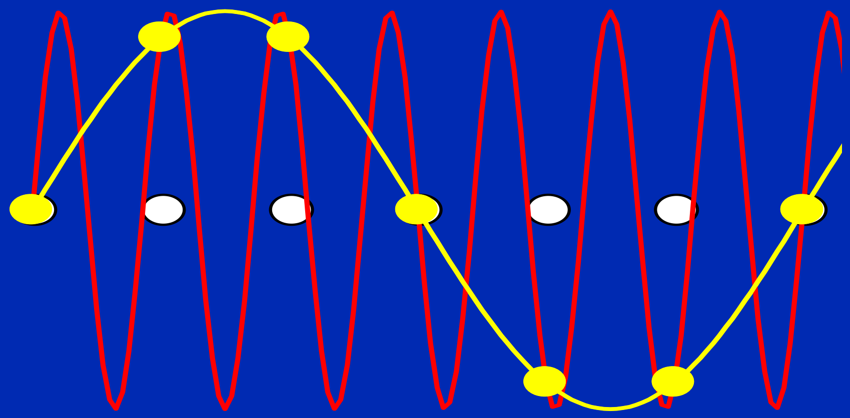


$$H = T + U = \sum_i \frac{p_i^2}{m_i} + \frac{1}{2}\sum_{<ij>} C_j (u_i - u_j)^2$$



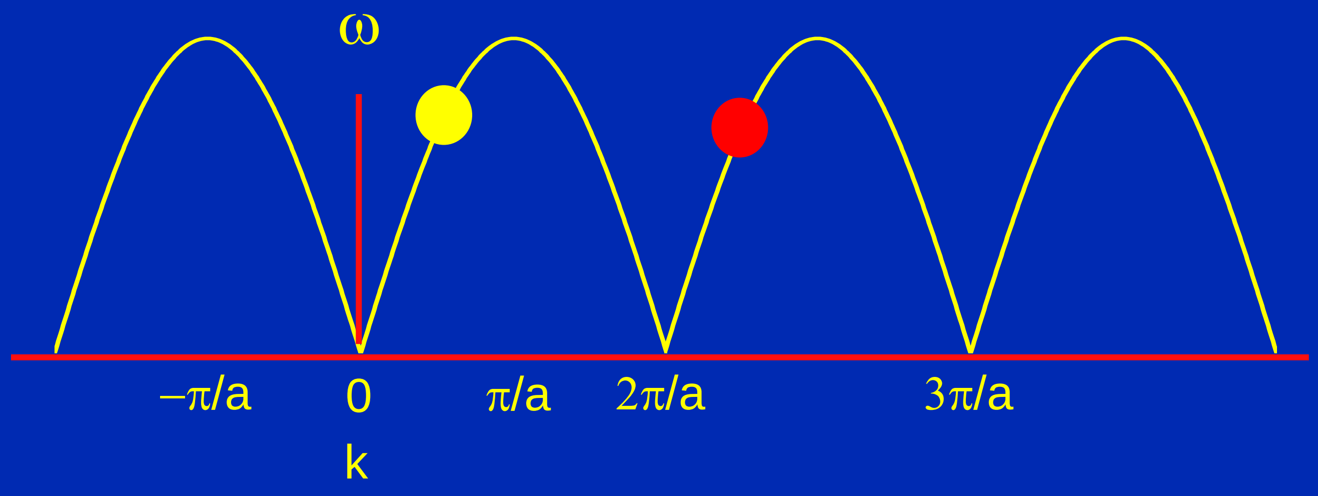
$$\omega(k) = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

Relevant values of k

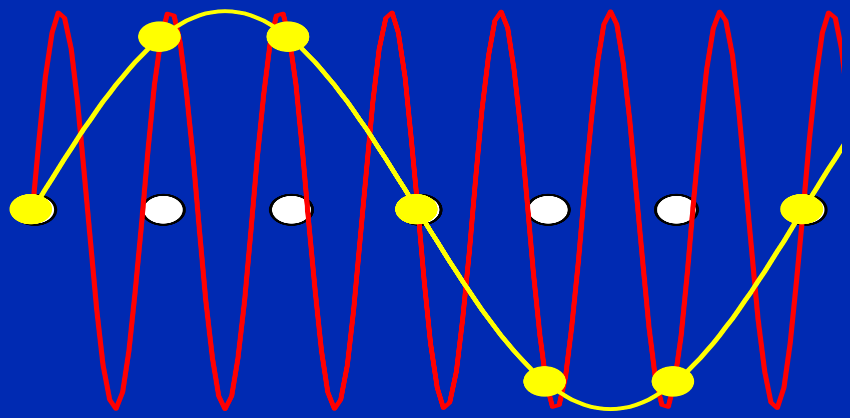


$$e^{i\left(\omega t - \frac{\pi}{3a} r\right)}$$

$$e^{i\left(\omega t - \frac{7\pi}{3a} r\right)}$$



Relevant values of k



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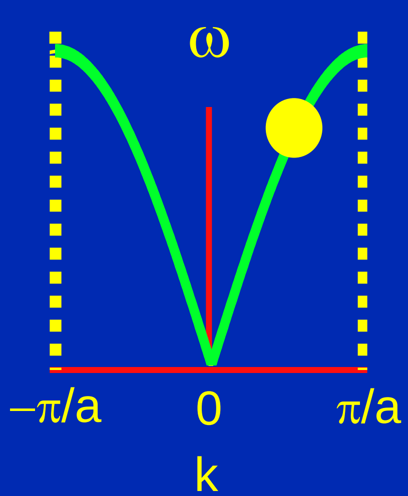
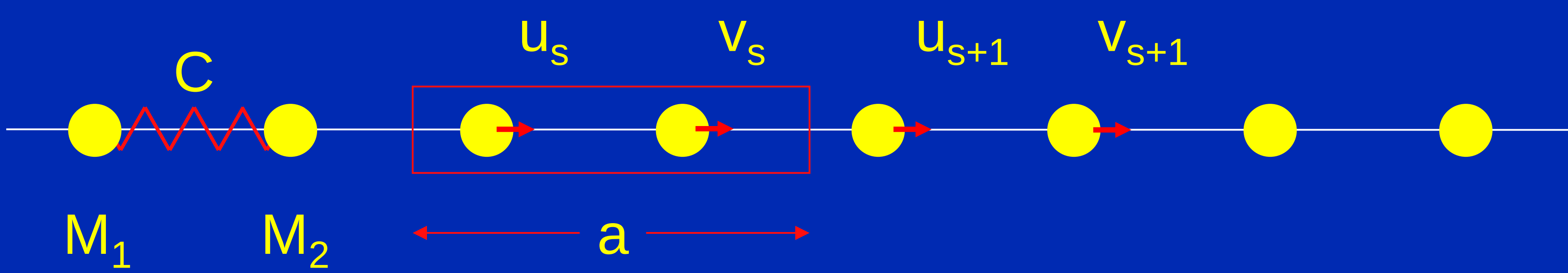


$$-\frac{\pi}{a} < k \le \frac{\pi}{a}$$

FIRST BRILLOUIN ZONE

1 dimensional -- 2 at./cell



EOM

$$M_1 \ddot{u}_s = -C\left(2u_s - v_s - v_{s-1}\right)$$

$$M_2 \ddot{v}_s = -C\left(2v_s - u_s - u_{s+1}\right)$$

Traveling wave

$$u_s(t) = u \cdot e^{ikas} \cdot e^{-i\omega t}$$

$$v_s(t) = v \cdot e^{ikas} \cdot e^{-i\omega t}$$

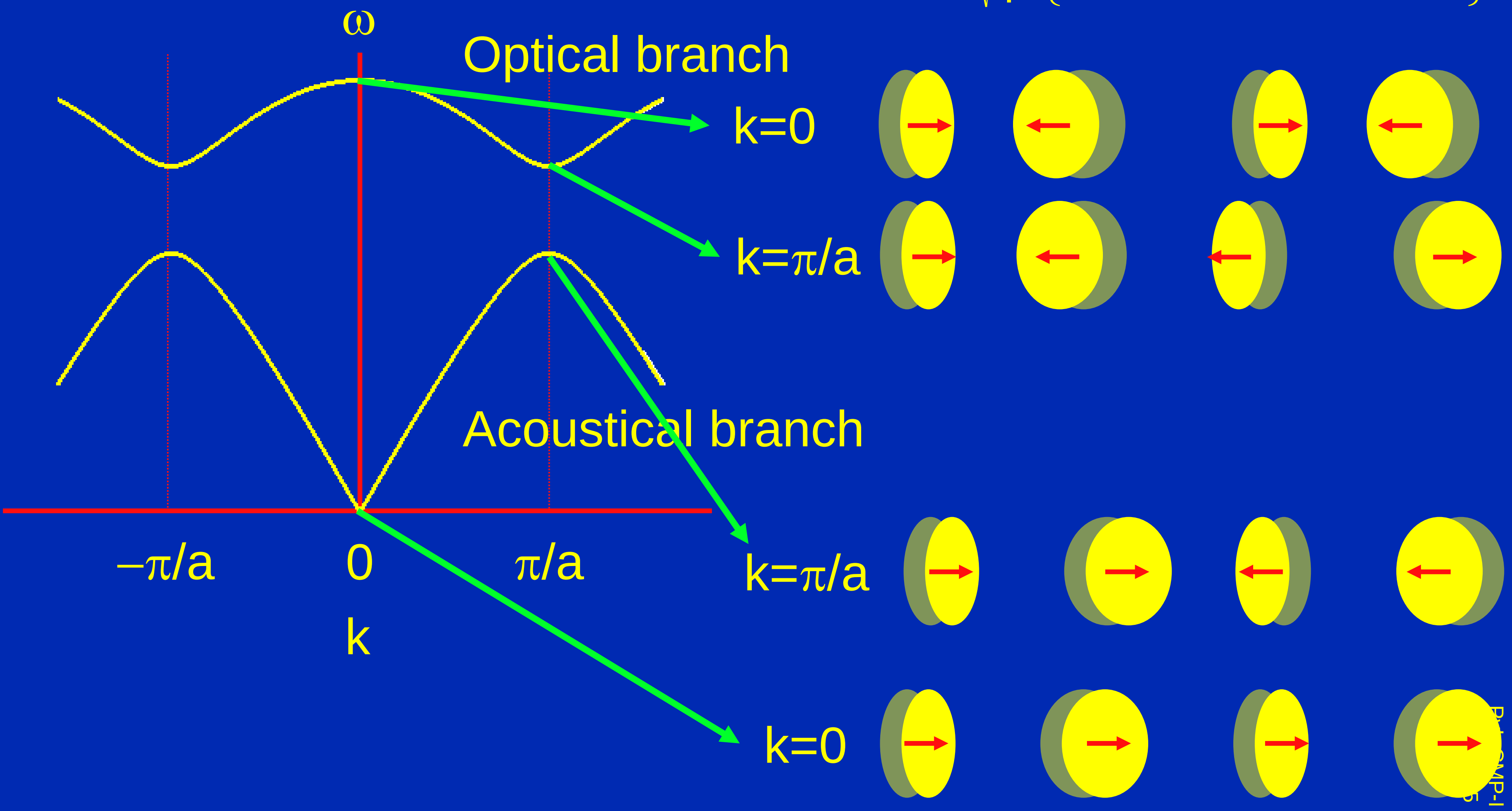
Dispersion

$$\omega^2(k) = \frac{C}{\mu}\left\{1 \pm \sqrt{1 - \frac{4\mu}{M}\sin^2(ka/2)}\right\}$$

$$\mu = \frac{1}{M_1} + \frac{1}{M_2}; \quad M = M_1 + M_2$$

Dispersion

$$\omega(k) = \sqrt{\frac{C}{\mu}\left\{1 \pm \sqrt{1 - \frac{4\mu}{M}\sin^2(ka/2)}\right\}}$$



Relevant values for k

$$\omega(k) = \sqrt{\frac{C}{\mu}\left\{1 \pm \sqrt{1 - \frac{4\mu}{M}\sin^2(ka/2)}\right\}}$$

<u>Solutions for **k** and for **k+h·2π/a**</u>

have the same frequency

$$\sin(\frac{ka}{2}) = \sin(\frac{ka}{2} + h \cdot 2\pi) \Rightarrow \omega(k + h\frac{2\pi}{a}) = \omega(k)$$

have the same wavefunctions

$$u_{k+h\cdot 2\pi/a}(s,t) = u \cdot e^{ikas} \cdot e^{i(h\cdot 2\pi/a)as} \cdot e^{-i\omega t} = u_k(s,t)$$

<u>Are identical</u>

Group velocity

$$v_g = \frac{\partial\omega(k)}{\partial k} \qquad \omega(k) = \sqrt{\frac{C}{\mu}\left\{1 \pm \sqrt{1 - \frac{4\mu}{M}\sin^2(ka/2)}\right\}}$$

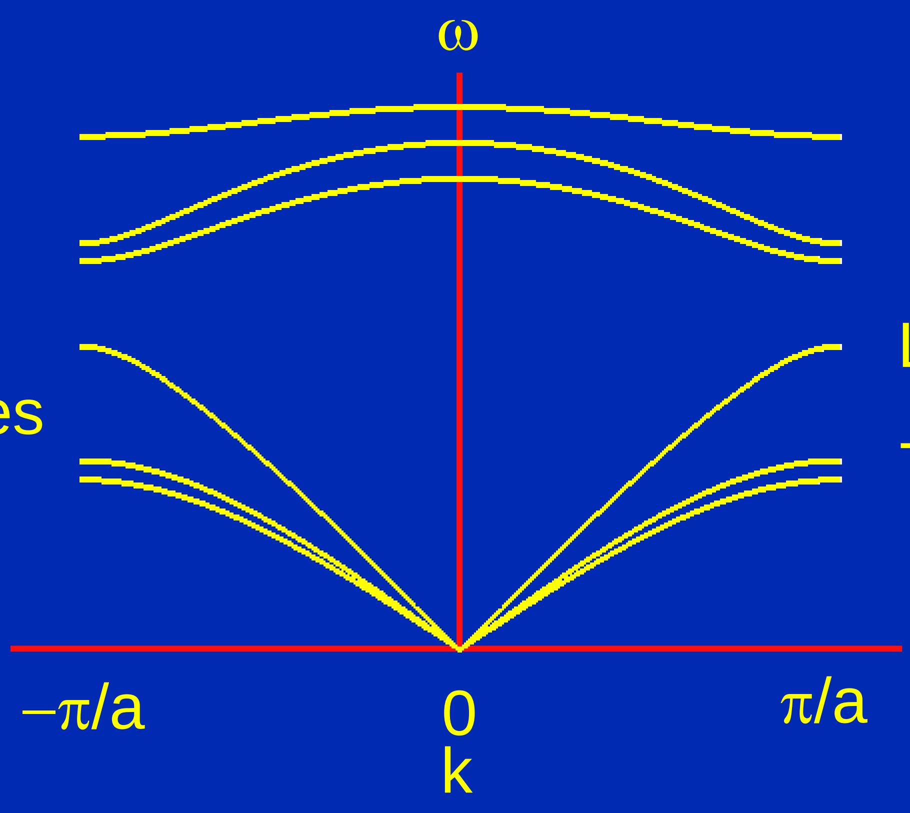
$k \approx 0$ $\quad \omega(k) = \sqrt{\frac{2C}{M}} \cdot \frac{ka}{2}$ $\quad v_g = \sqrt{\frac{2C}{M}}\frac{a}{2}$ $\quad$ <u>Sound velocity</u> $\omega = v_g \cdot k$

$\omega(k) = \sqrt{\frac{2C}{\mu}}$ $\quad v_g = 0$

$k \approx \pm\pi/a$ $\quad \omega(k) \approx$ constant: Standing wave

Three dimensions

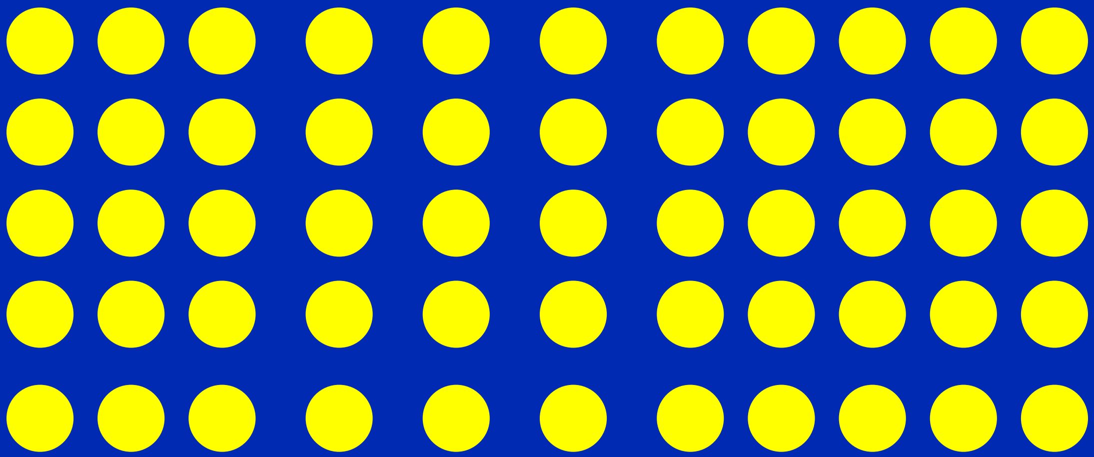
3-dimensional crystal:	3 degrees of freedom per atom
s atoms per primitive cell:	3 acoustical branches
	3*s*-3 optical branches



Sound waves

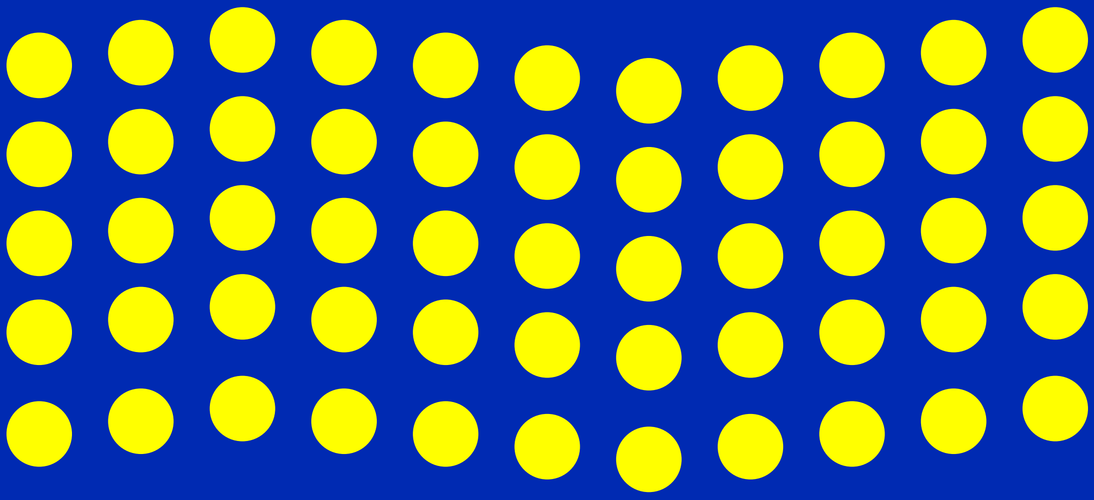
Longitudinal
Acoustical

u // k



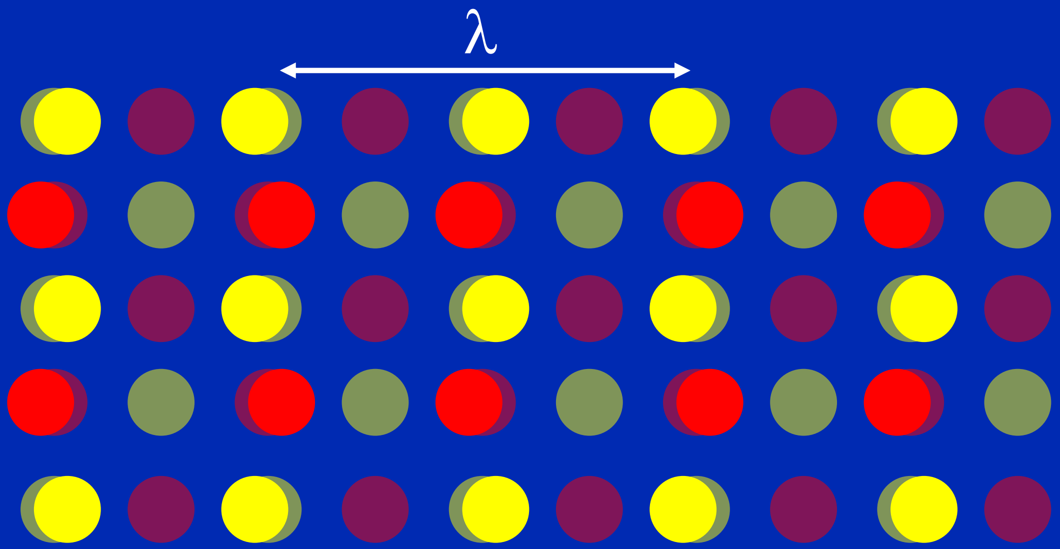
Transverse
acoustical

u ⊥ k

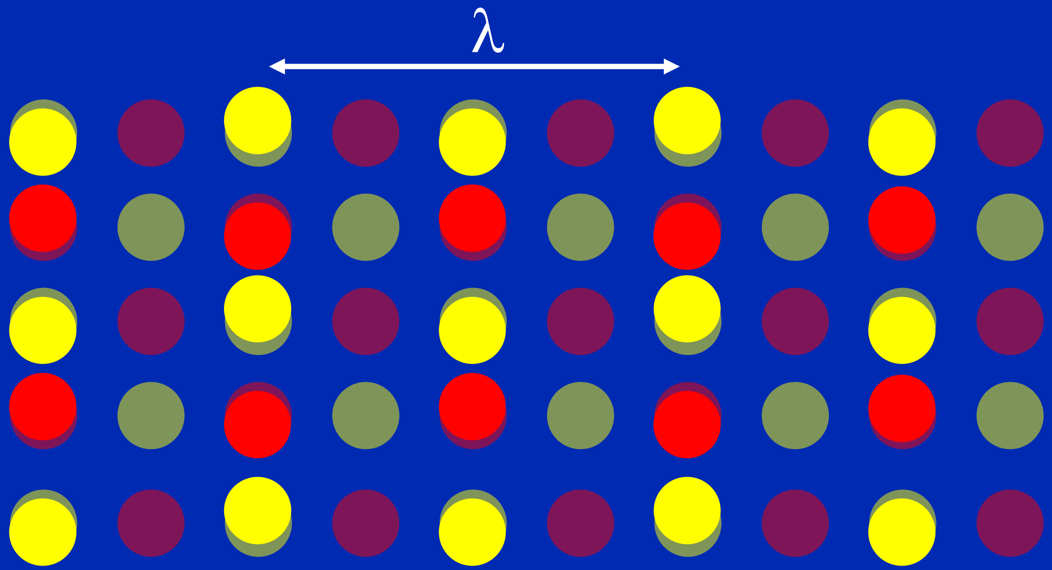


Optical waves

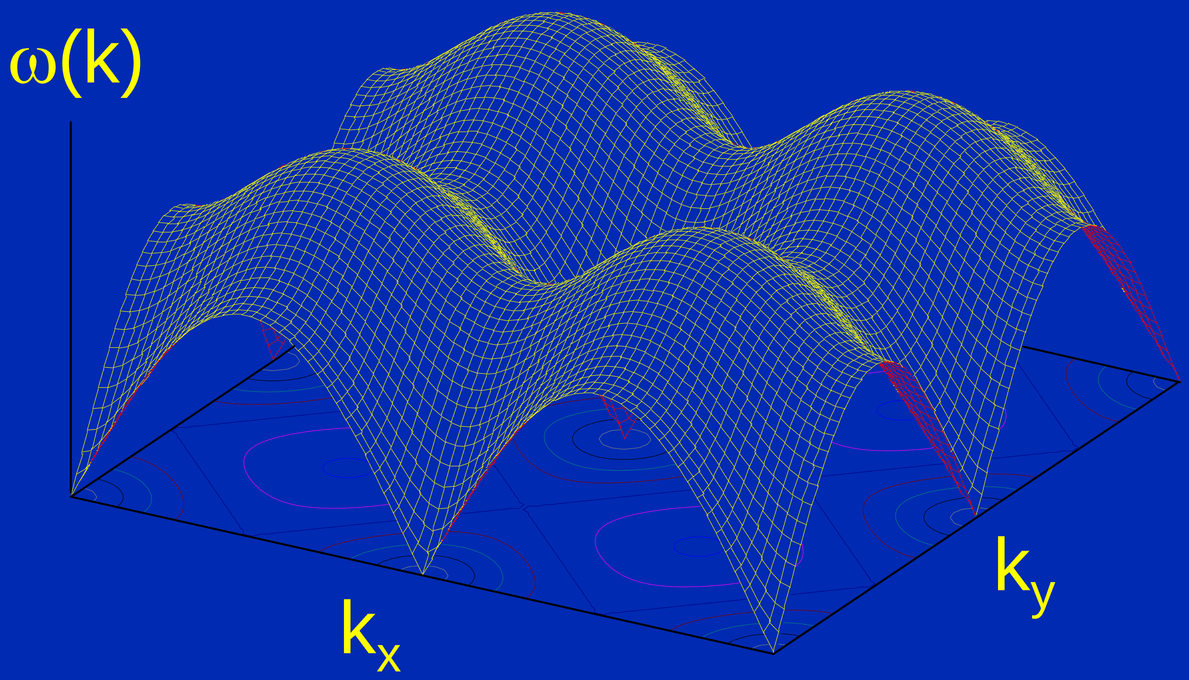
Longitudinal
optical phonons



Transversal
optical phonons



Dispersion in two dimensions



$$\omega_k = \sqrt{\frac{4C}{m}}\sqrt{\sin^2\left(\frac{k_x a}{2}\right)+\sin^2\left(\frac{k_y a}{2}\right)}$$

phonons

Classical: $u_s(t) = u_k(t)\, e^{i\,kas}$

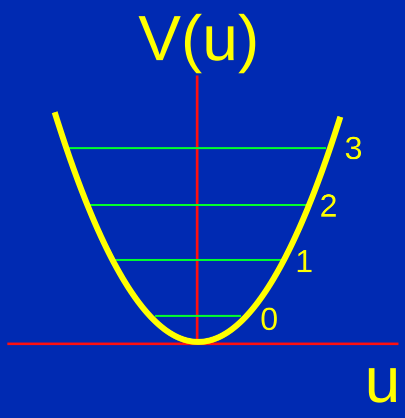
EOM: $m\ddot{u}_k(t) = -C_k u_k(t)$ with $C_k = m\omega_k^{\,2}$

Quantum states of elastic waves:

$$\left\{-\frac{\hbar}{2m}\frac{\partial^2}{\partial u_k^{\,2}} + \frac{1}{2}m\omega_k^{\,2}u_k^{\,2}\right\}\cdot\psi_k(u_k) = E_k\cdot\psi_k(u_k)$$

$$\psi_k(u_k,t) = e^{i(E_k/\hbar)t}\cdot\psi_k(u_k)$$

$$E_k = (n + \frac{1}{2})\cdot\hbar\omega_k$$



See kittel appendix C: quantization of elastic waves: phonons

Properties of phonons

Any number can occupy the same vibrational mode u_k

⇨ Phonons are *bosons*

⇨ Thermal occupation given by Planck's distribution

$$\langle n_k \rangle = \frac{1}{e^{(\hbar\omega_k / k_b T)} - 1}$$

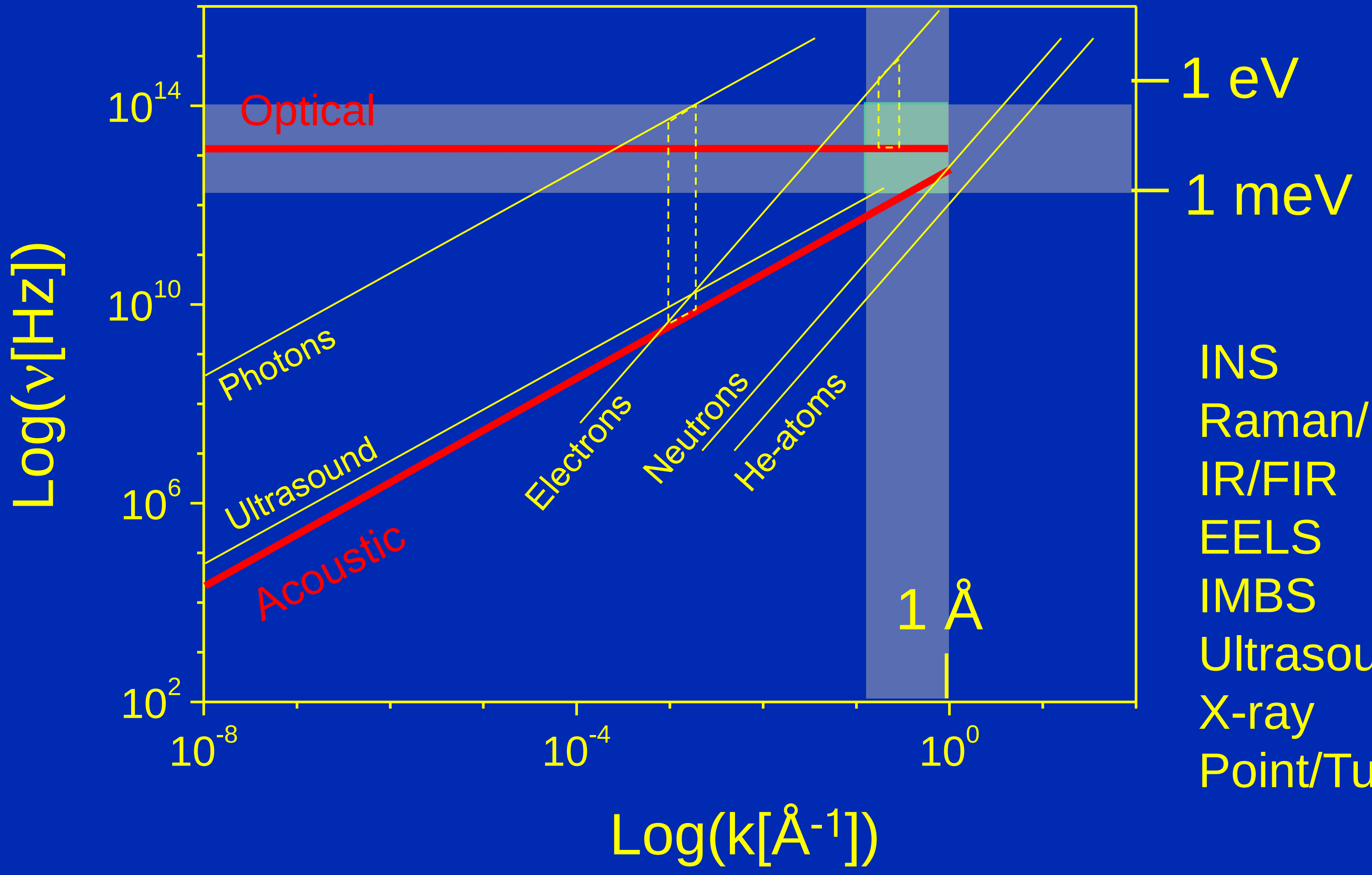
Zero-point energy: $E_0 = \sum_k \frac{1}{2}\hbar\omega_k$

Energy of 1 phonon: $\hbar\omega_k$

"Momentum" of 1 phonon: $\hbar k$

Phonons: *Quantum excitations* of solids

Measuring phonons

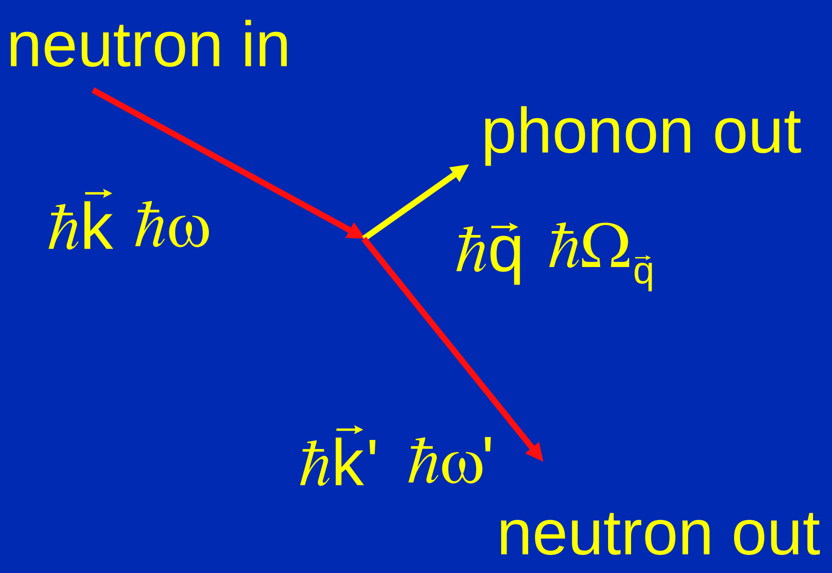


INS
Raman/Brillouin
IR/FIR
EELS
IMBS
Ultrasound
X-ray
Point/Tunnel

Phonon momentum

Total momentum of a crystal with phonon k is zero !

$$P = M\frac{\partial}{\partial t}\sum_{s}^{N} u_s = M\frac{\partial u}{\partial t}\cdot\sum_{s} e^{ikas} = M\frac{\partial u}{\partial t}\cdot\frac{1-e^{ikaN}}{1-e^{ika}} = 0$$



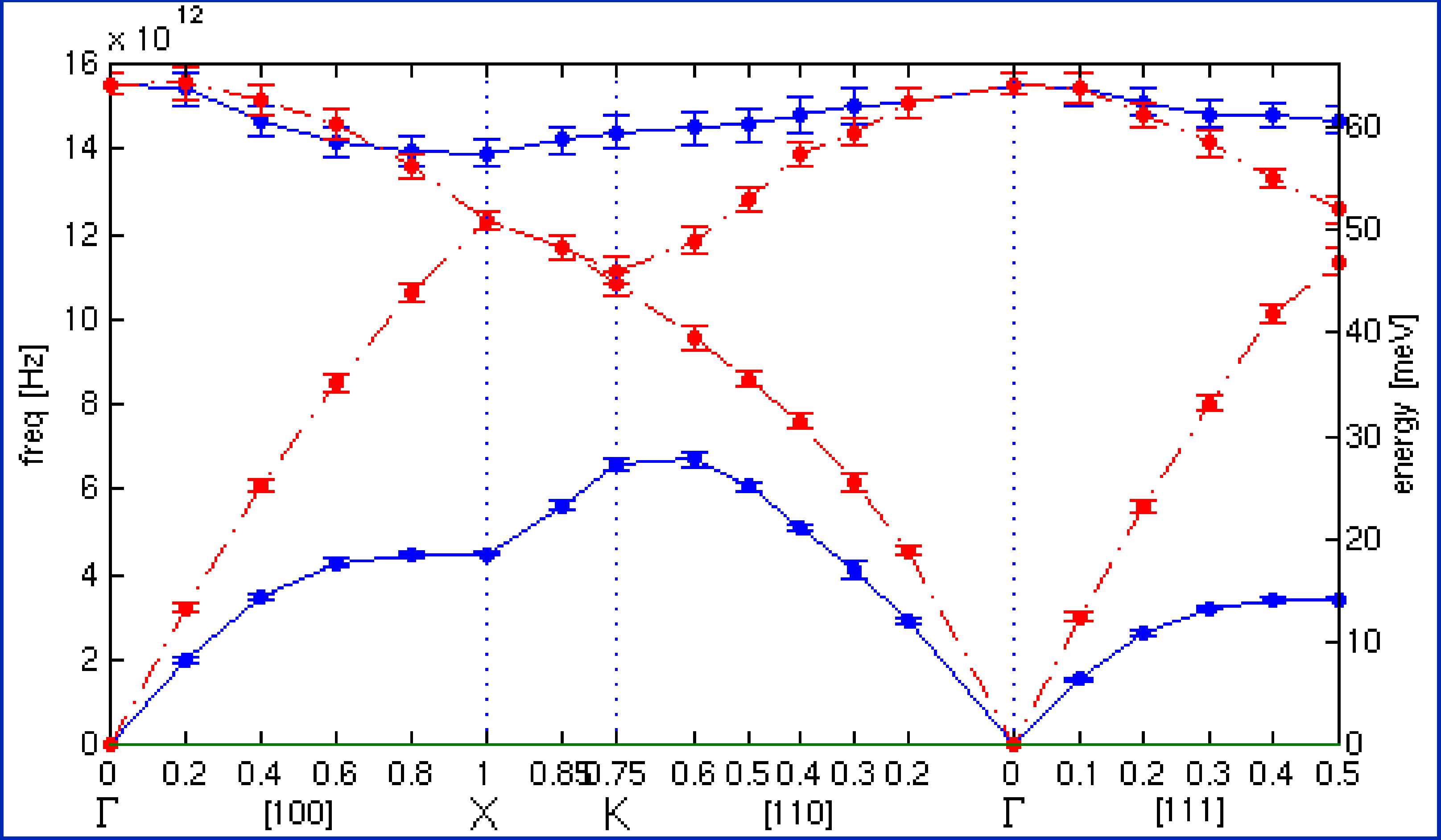
Energy conservation

$$\frac{\hbar^2 k^2}{2m_n} = \frac{\hbar^2 k'^2}{2m_n} \pm \hbar\Omega$$

“Momentum” conservation

$$k = k' \pm q + G$$

Phonon dispersion in Si



Inelastic phonon scattering

- Polarization response $P = \varepsilon_0 \chi E$
- Phonons modulate susceptibility

$$P(t) = \varepsilon_0 \chi(t) E(t); \qquad E(t) = E_0 \cos(\omega t)$$

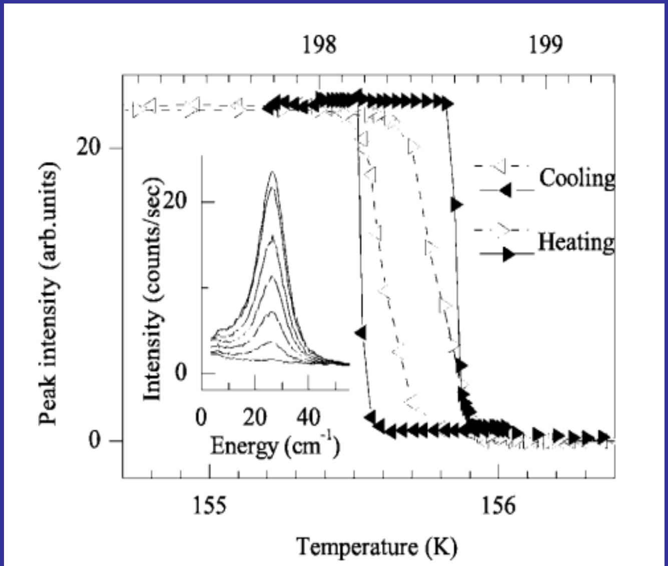
$$\chi = \chi_0 + \frac{d\chi}{dQ} Q = \chi_0 + \chi' \cos(\Omega t)$$

$$P(t) = \varepsilon_0 \chi_0 E_0 \cos(\omega t) + \varepsilon_0 \chi' \cos(\Omega t) E_0 \cos(\omega t)$$

$$= \varepsilon_0 \chi_0 E_0 \cos(\omega t) + \frac{1}{2} \varepsilon_0 \chi' E_0 \left[\cos([\omega + \Omega]t) + \cos([\omega - \Omega]t)\right]$$

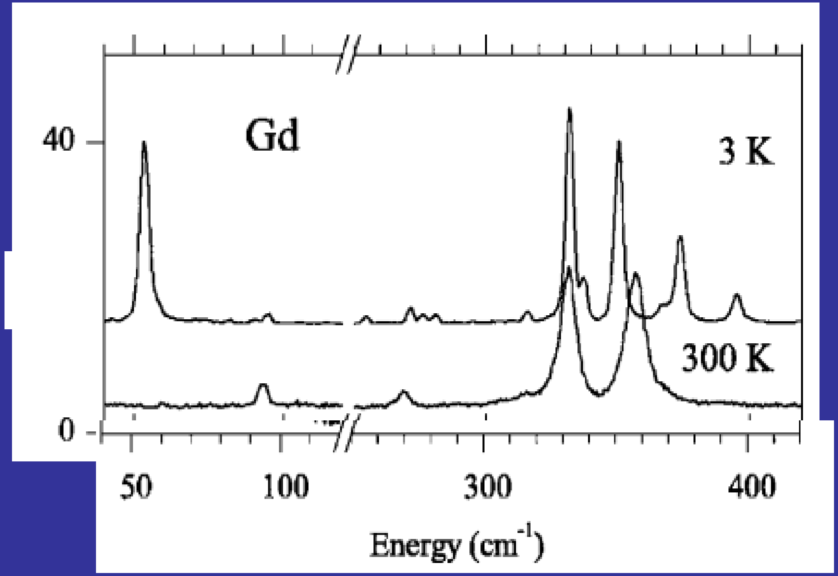
- Dipole radiation at ω, and $\omega \pm \Omega$
- Rayleigh scattering and Raman sidebands
- Ratio anti-Stokes and Stokes intensity $\frac{I_{anti-stokes}}{I_{stokes}} = e^{-\frac{\hbar\Omega}{kT}}$

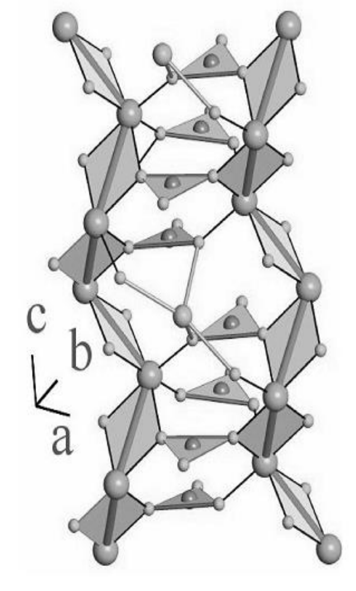
Raman scattering



Vibrational spectroscopy

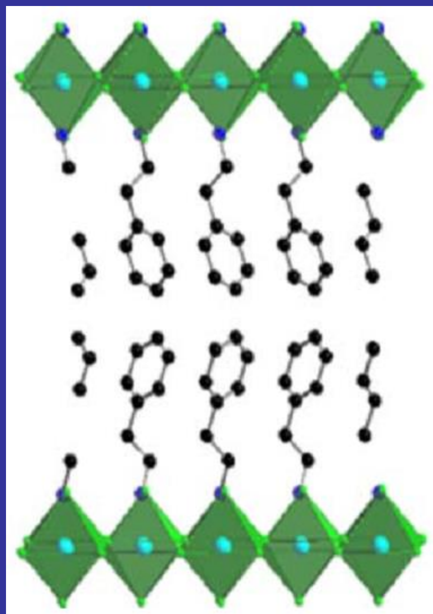
- Symmetry
- Phase transitions
- Coupling to other excitations
- Bond specific (chemical composition)
- Temperature (ratio stokes/ant-stokes)
-
-

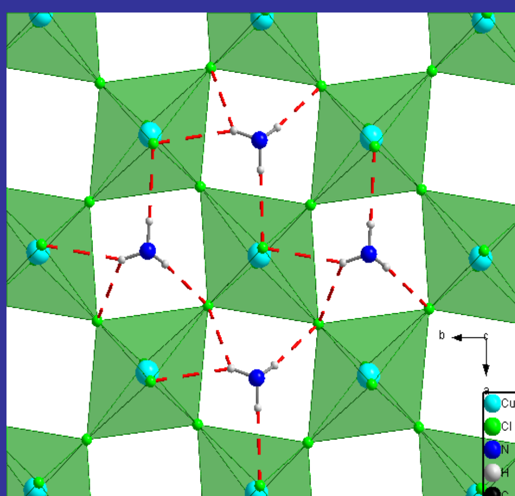


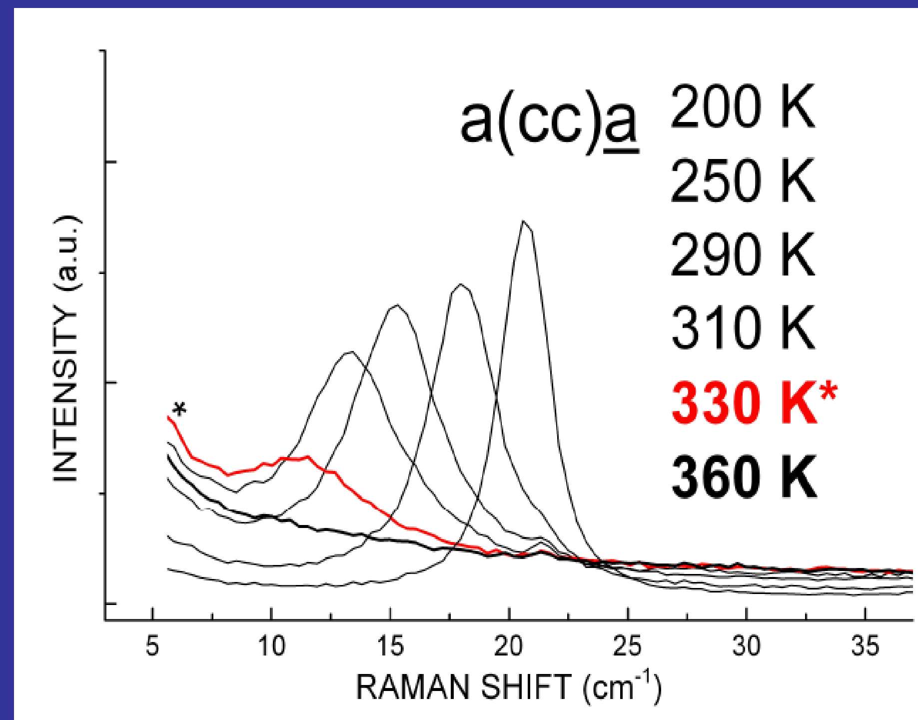


First order phase transition in $RFe_3(BO_3)_4$
D. Fausti et al., PRB **74**, 024403 1996

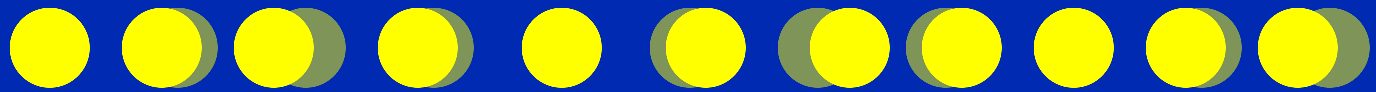
Hybrids: Orientational melting



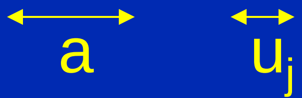




Harmonic crystal:
No thermal expansion



$$r_j = ja + u_j$$

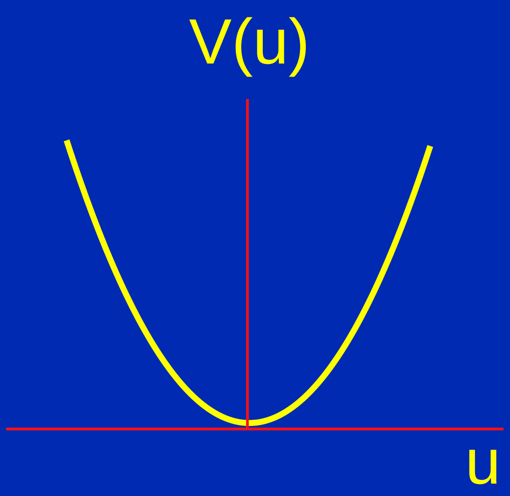


Harmonic

$$V(u_j) = \alpha \cdot u_j^{\,2}$$

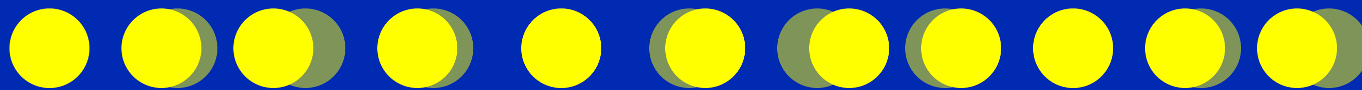
$$a(T) = a + \langle u_j \rangle_T = a$$

$$\langle u_j \rangle_T = \frac{\int du \cdot u\, e^{-V(u_j)/k_B T}}{\int du \cdot e^{-V(u_j)/k_B T}} = 0$$



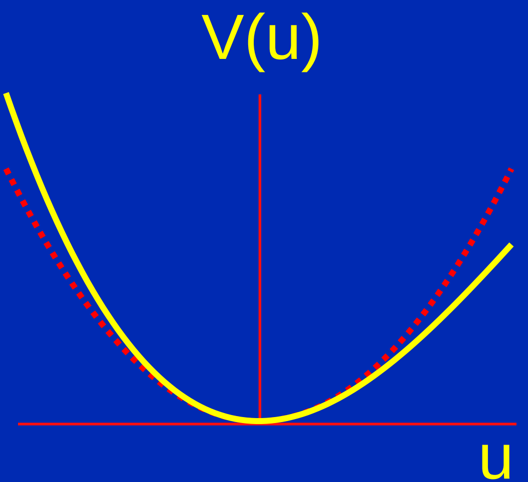
No lattice expansion !!

Anharmonicity:
Thermal expansion (classical)



$$r_j = ja + u_j \qquad a \qquad u_j$$

Weak anharmonicity



$$V(u_j) = \alpha \cdot u_j^{\,2} - \gamma \cdot u_j^{\,3}$$

$$\langle u_j \rangle_T = \frac{\int du \cdot u\, e^{-V(u_j)/k_B T}}{\int du \cdot e^{-V(u_j)/k_B T}} \approx \frac{3/4\,(k_B T)^{3/2}\sqrt{\pi}\,\gamma\,\alpha^{-5/2}}{\sqrt{k_B T}\sqrt{\pi}\,\alpha^{-1/2}}$$

$$a(T) = a_0 + \langle u_j \rangle_T = a_0 + \frac{3\gamma}{4\alpha^2} k_B T$$

Lattice expansion is caused by anharmonicity !