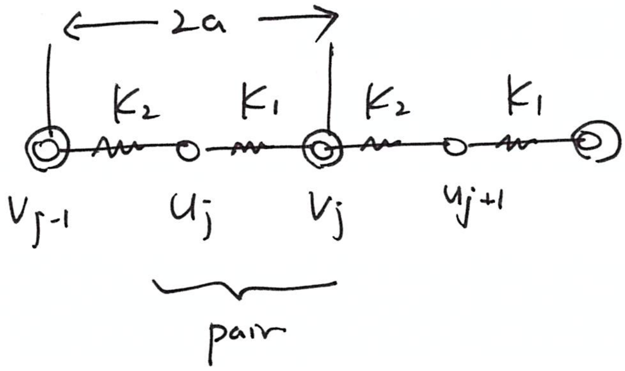
- Phonon with basis atom



$$F_j^u = K_1(v_j - u_j) + K_2(v_{j-1} - u_j) = m\frac{d^2u_j}{dt^2}$$

$$F_j^v = K_2(u_{j+1} - v_j) + K_1(u_j - v_j) = m\frac{d^2v_j}{dt^2}.$$

$$u_j(t) = u_q e^{iqr_j} e^{-i\omega t} \qquad r_j = (2a)j \qquad u \text{ atoms}$$

$$v_j(t) = v_q e^{iqr_j} e^{-i\omega t} \qquad = 2a(j+\tfrac{1}{2}) \qquad v \text{ atoms}$$

$$m(-i\omega_q)^2 u_j(t) = e^{-i\omega_q t} e^{iq2aj}\left[(e^{iqa}v_q - u_q)K_1 + (e^{-iqa}v_q - u_q)K_2\right]$$

$$-m\omega_q^2 u_q = (K_1 e^{iqa} + K_2 e^{-iqa})v_q - (K_1+K_2)u_q$$

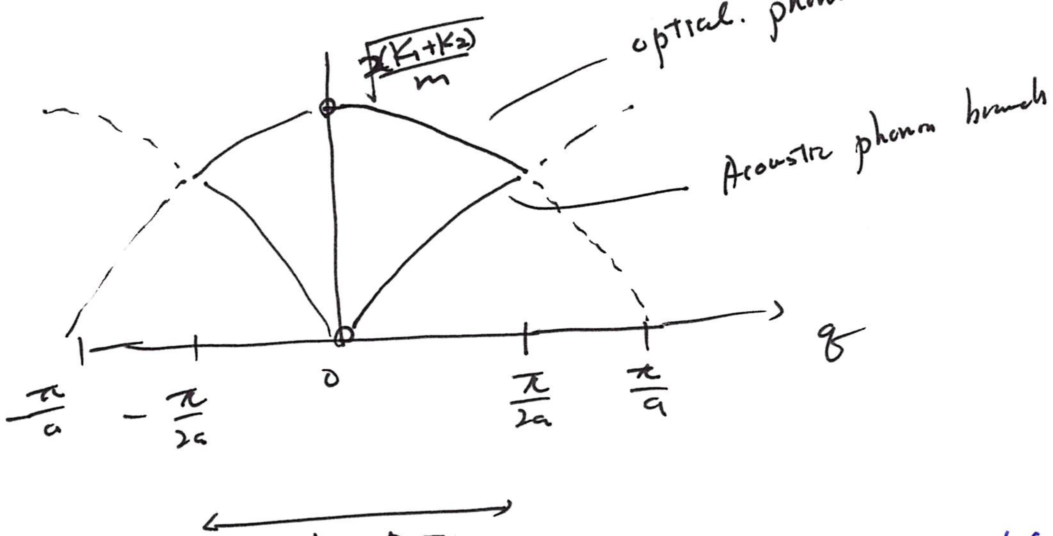
$$-m\omega_q^2 v_q = (K_2 e^{iqa} + K_1 e^{-iqa})u_q - (K_1+K_2)v_q$$

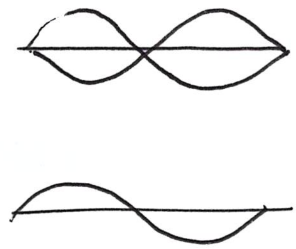
$$\det\begin{bmatrix} m\omega_q^2 - (K_1+K_2) & K_1 e^{iqa} + K_2 e^{-iqa} \\ K_2 e^{iqa} + K_1 e^{-iqa} & m\omega_q^2 - (K_1+K_2)\end{bmatrix} = 0$$

$$\rightarrow [m\omega_q^2 - (K_1+K_2)]^2 - (K_1^2 + K_2^2 + 2K_1K_2\cos 2qa) = 0$$

$$m\omega_q^2 = (K_1+K_2) \pm \sqrt{K_1^2+K_2^2+2K_1K_2\cos 2qa}$$

$$\therefore\ \omega_q = \left\{ \frac{K_1 + K_2}{m} \pm \frac{1}{m}\sqrt{K_1^2 + K_2^2 + 2K_1K_2\cos 2qa} \right\}^{1/2}.$$





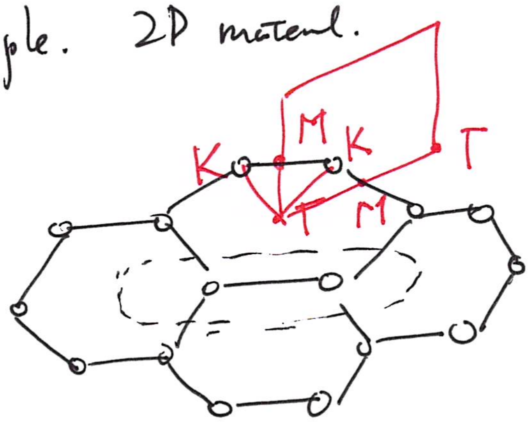
1st B.Z.

cell of 2a. (1 basis)
w/

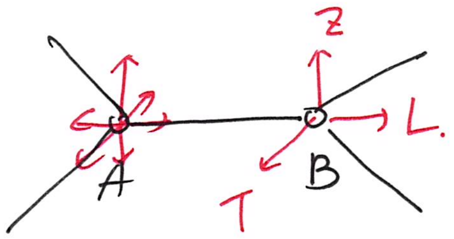
$K = \frac{2\pi}{\lambda}$, $\omega = 2\pi\nu$

velocity $= \frac{\omega}{K} = \nu \cdot \lambda$.

Example. 2D material.



two carbon atoms (A, B)
in one unit cell.



phonon dispersion

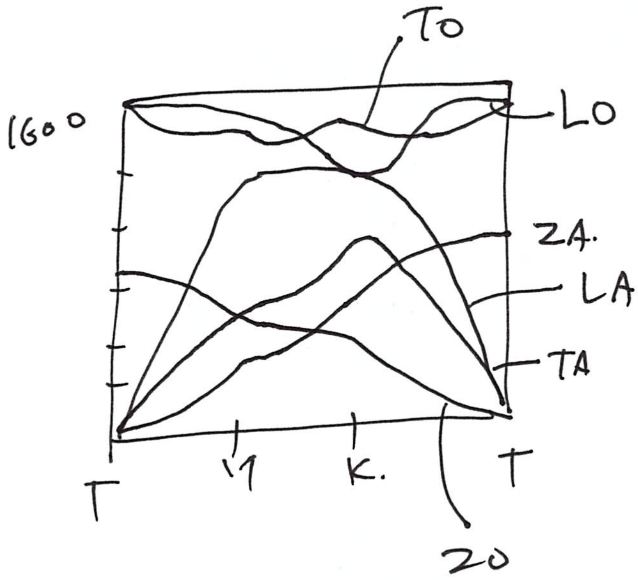
3 Acoustic branches } Z L T

3 optical branches. } Z L T

Z : out-of-plane

L : in-plane longitudinal

T : in-plane transverse

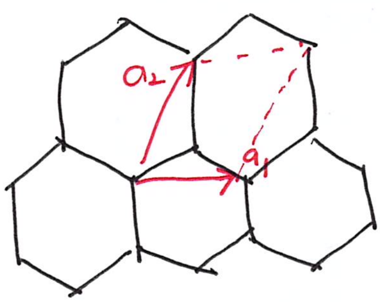


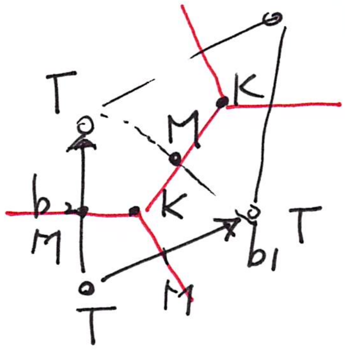
Raman spectrum.

Raman } selection rule
FTIR }

↓

study.

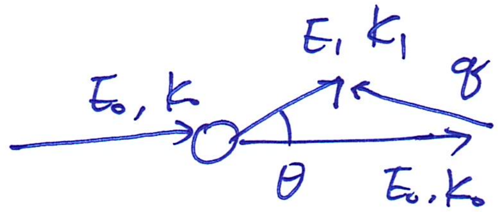


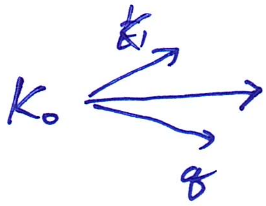


* How to measure Phonon.

Inelastic scattering

Raman scattering or spectroscopy





$$\vec{K}_0 = \vec{k}_1 - \vec{q}$$

Measurement of dispersion relations
coming down to the dependence of the energy
of scattered wave-particles (photons, neutrons) on the angle
under the scattering occurs.

Quasi-Harmonic Approximation

$$C_V(T) = \frac{1}{V}\frac{\partial E}{\partial T}$$

partition fn. Z_i

$$Z_i = \sum_j e^{-\varepsilon_j(\omega_i)/k_B T}$$

$$= \frac{e^{-\hbar\omega_i/2k_BT}}{1 - e^{-\hbar\omega_i/k_BT}}$$

$$F_i^{th} = -k_BT \ln Z_i$$

$$= \frac{1}{2}\hbar\omega_i + k_BT \ln(1 - e^{-\hbar\omega_i/k_BT})$$

$$F = E + \sum_i F_i^{th}$$

$$= \underbrace{U}_{\text{zero-temp energy}} + \underbrace{\frac{1}{2}\sum \hbar\omega}_{\text{zero-point energy}} + \underbrace{k_BT \sum_i \ln(1 - e^{-\hbar\omega_i/k_BT})}_{\text{temp. contribution to } E.}$$

$$B \equiv V\left(\frac{\partial^2 U}{\partial V^2}\right)_{p,T}$$