

Monatomic basis \rightarrow 3 modes of vibration
 1 longitudinal, 2 Transverse.

Polyatomic basis \Rightarrow new dispersion relation feature

e.g. 2 atom basis \Rightarrow 2 branches for each mode of vibration.

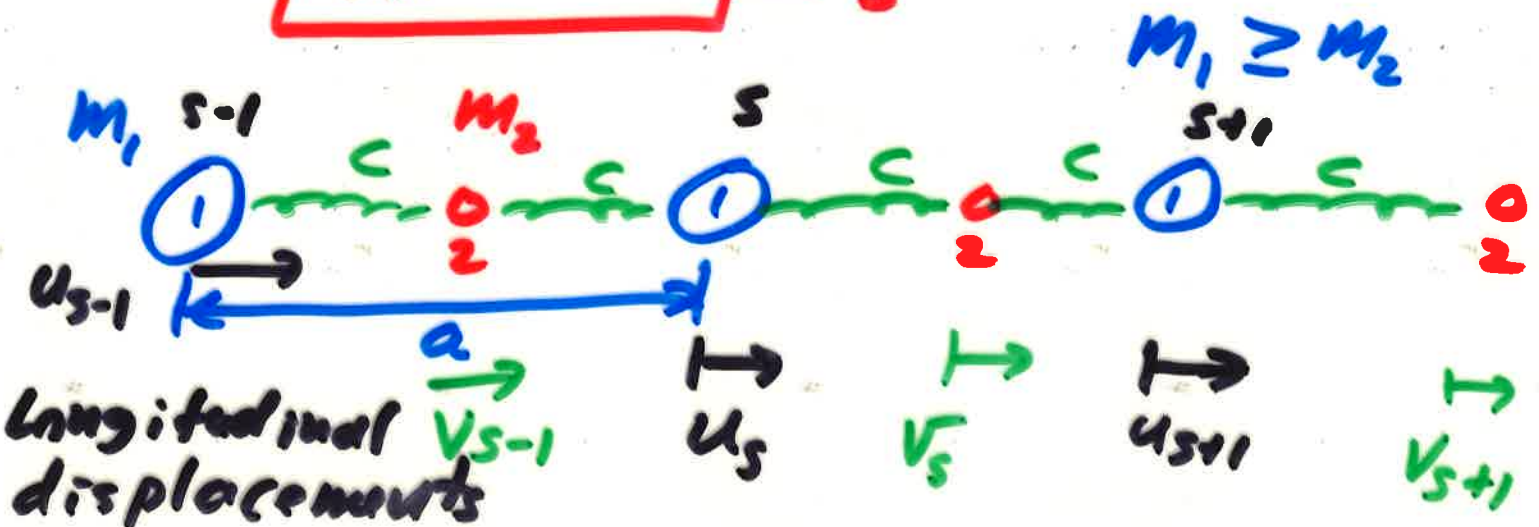
LO 2TO } 6 total
LA 2TA } 3

L - Longitudinal
 O - optical

T - transverse
 A - acoustic

e.g. 3 atom basis \Rightarrow 3 branches per mode

2LO 4TO } 9 total
LA 2TA } 3



$$\textcircled{1} m_1 \frac{d^2 u_s}{dt^2} = C [v_{s-1} - u_s] + C [v_s - u_s]$$

$$= C [v_{s-1} + v_s - 2u_s]$$

$$m_2 \frac{d^2 v_s}{dt^2} = C [u_s - v_s] + C [u_{s+1} - v_s]$$

$$= C [u_s + u_{s+1} - 2v_s]$$

Look for wave-like solutions.
 (Take Fourier space and time
 + transforms.) a.s = x

$$u_s = A e^{i(kas - \omega t)}$$

$$v_s = B e^{i(kas - \omega t)}$$

$e^{i(kas - \omega t)} \sim e^{i(kx - \omega t)}$ right moving wave
 Look at point in wave with
 zero phase.

$$-\omega^2 A m_1 = c B [1 + e^{-ika}] - 2c A$$

$$-\omega^2 B m_2 = c A [e^{+ika} + 1] - 2c B$$

$$(2c - \omega^2 m_1) A - c [1 + e^{-ika}] B = 0$$

$$-c [e^{+ika} + 1] A + (2c - \omega^2 m_2) B = 0$$

$$\begin{bmatrix} 2c - \omega^2 m_1 & -c(1 + e^{-ika}) \\ -c(e^{+ika} + 1) & 2c - \omega^2 m_2 \end{bmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\equiv \underline{\underline{M}} \cdot \underline{\underline{v}} = \underline{\underline{0}}$$

If $\underline{\underline{M}}$ had an inverse: $\underline{\underline{M}}^{-1} \underline{\underline{M}} \cdot \underline{\underline{v}} = \underline{\underline{M}}^{-1} \underline{\underline{0}}$

$$\Rightarrow \underline{\underline{I}} \cdot \underline{\underline{v}} = \underline{\underline{v}} = \underline{\underline{0}} \Rightarrow A=0, B=0$$

Non-trivial solutions

~~$\underline{\underline{M}}^{-1}$~~

$$\underline{\underline{I}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\underline{\underline{M}}^{-1} = \frac{1}{\det(\underline{\underline{M}})} \text{adj}(\underline{\underline{M}})$$

If $\det(\underline{\underline{M}}) = 0$ then there is no $\underline{\underline{M}}^{-1}$

$$\det(\underline{\underline{M}}) = (2c - \omega^2 m_1)(2c - \omega^2 m_2) - c^2(1 + e^{ika})(1 + e^{-ika}) = 0$$

$$\Rightarrow 4c^2 - 2c(\omega^2(m_1 + m_2)) + \omega^4 m_1 m_2 - c^2(2 + e^{ika} + e^{-ika}) = 0$$

$$\Rightarrow m_1 m_2 (\omega^2)^2 - 2c(m_1 + m_2) \omega^2 + 2c^2[1 - \cos(ka)] = 0$$

Quadratic equation in ω^2

$$a(\omega^2)^2 + b\omega^2 + c = 0$$

$$\omega^2 = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Reduced Mass

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$\mu < m_1, m_2$$

$$\omega^2 = c \left(\frac{1}{m_1} + \frac{1}{m_2} \right) \pm c \sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2} \right)^2 - \frac{4}{m_1 m_2} \sin^2\left(\frac{ka}{2}\right)}$$

$$\omega^2 = \frac{c}{\mu} \pm c \sqrt{\frac{1}{\mu^2} - \frac{4}{m_1 m_2} \sin^2\left(\frac{ka}{2}\right)}$$

Long wave length limit $ka \ll 1$

$$\cos(ka) = 1 - \frac{1}{2}k^2 a^2 + O(k^4) \dots$$

$$\det(\underline{M}) = \omega^4 m_1 m_2 - 2C(m_1 + m_2)\omega^2 + C^2 k^2 a^2 = 0$$

$$\omega^2 = \frac{2C(m_1 + m_2) \pm \sqrt{4C^2(m_1 + m_2)^2 - 4m_1 m_2 C^2 k^2 a^2}}{2m_1 m_2}$$

$$\oplus \omega^2 = \frac{2C(m_1 + m_2) + 2C(m_1 + m_2)}{2m_1 m_2} = 2C\left(\frac{1}{m_1} + \frac{1}{m_2}\right) = \frac{2C}{\mu} \text{ optical}$$

$$\ominus \omega^2 = \frac{2C(m_1 + m_2) - 2C(m_1 + m_2) \sqrt{1 - \frac{k^2 a^2 m_1 m_2}{(m_1 + m_2)^2}}}{2m_1 m_2}$$

Binomial expansion

$$\sqrt{1-x} = (1-x)^{\frac{1}{2}} \approx 1 - \frac{x}{2} + O(x^2) \dots$$

$$\omega^2 = \frac{2C(m_1 + m_2) k^2 a^2 m_1 m_2}{2(m_1 + m_2)^2 m_1 m_2} = \frac{C k^2 a^2}{2(m_1 + m_2)} \text{ acoustic}$$

acoustic mode ; M_{total}
(symmetric)



Center of mass moves

optical mode ; μ -reduced mass
(antisymmetric)



Center of mass stays fixed

At the Brillouin zone Boundary
 $ka = \pm \pi$

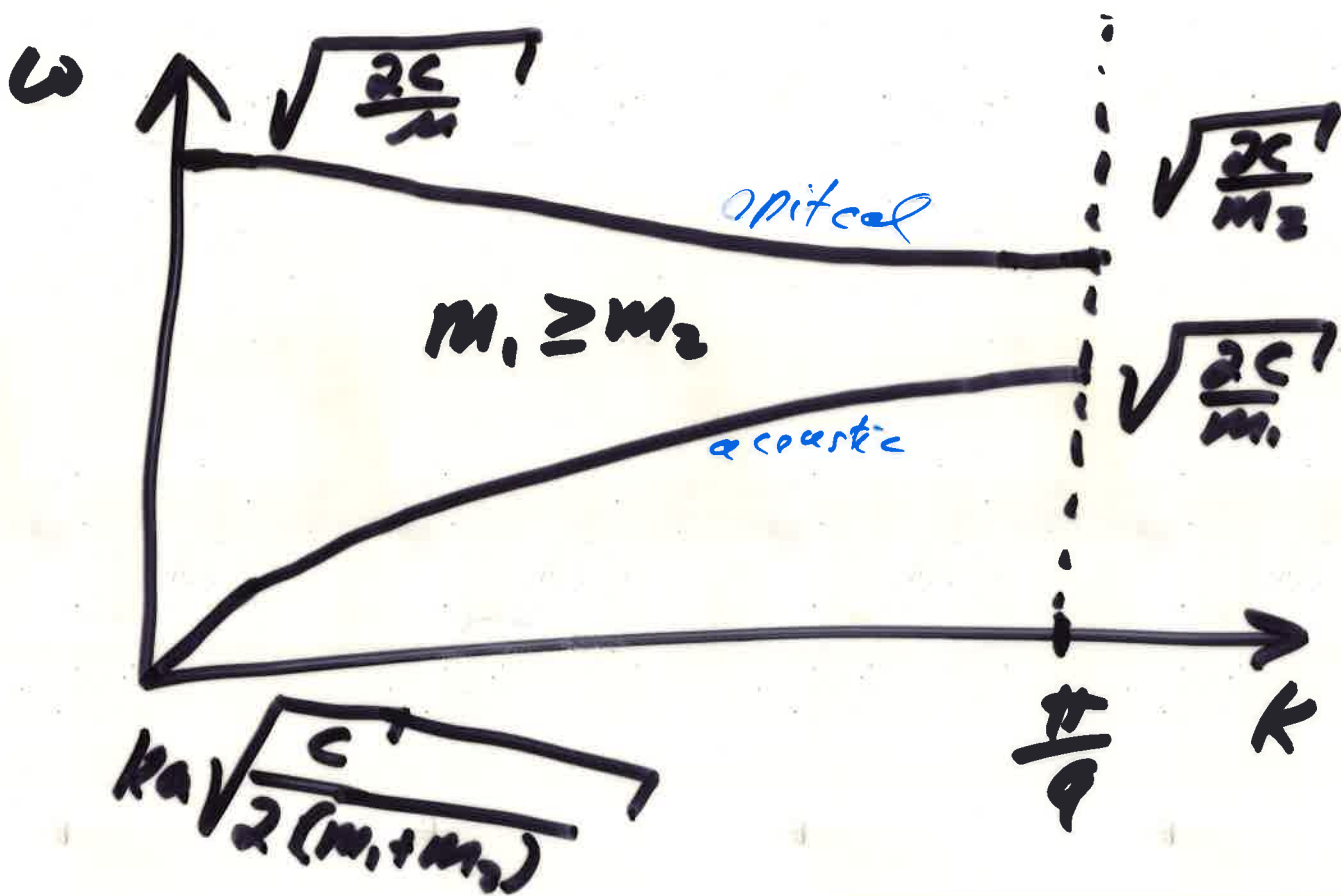
$$\cos(ka) \Rightarrow \cos(\pm\pi) = -1$$

$$\det(M) = \omega^4 m_1 m_2 - 2C(m_1 + m_2)\omega^2 + 4C^2 = 0$$

$$\Rightarrow \omega^2 = \frac{2C(m_1 + m_2) \pm \sqrt{4C^2(m_1 + m_2)^2 - 16C^2 m_1 m_2}}{2 m_1 m_2}$$

$$\oplus \omega^2 = \frac{2c}{m_2}$$

$$\ominus \omega^2 = \frac{2c}{m_1}$$



Why "optical" If crystal is ionic



Visible light 4000-7000 Å

