Phonons - continued

$$\omega^2 = \frac{c(m_1+m_2) \pm c\sqrt{m_1^2+m_2^2+2m_1m_2\cos(ka)}}{m_1m_2}$$

$m_1^2+m_2^2+2m_1m_2\cos(ka)+2m_1m_2-2m_1m_2 =$

$(m_1^2+m_2^2+2m_1m_2)+2m_1m_2[\cos(ka)-1]$

$=(m_1+m_2)^2+2m_1m_2[\cos(ka)-1]$

$=(m_1+m_2)^2\left\{1+\frac{2m_1m_2}{(m_1+m_2)^2}[\cos(ka)-1]\right\}$

In the long wavelenght limit, $k=\frac{2\pi}{\lambda} \ll 1$

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

$=(m_1+m_2)^2\left\{1+\frac{2m_1m_2}{(m_1+m_2)^2}\left(-\frac{k^2a^2}{2}\right)\right\} = (m_1+m_2)^2\left(1-\frac{m_1m_2k^2a^2}{(m_1+m_2)^2}\right)$

$$\omega^2 = \frac{c(m_1+m_2) \pm c(m_1+m_2)\sqrt{1-x}}{m_1m_2} \qquad x=\frac{m_1m_2k^2a^2}{(m_1+m_2)^2}$$

$\sqrt{1-x} \approx 1-\frac{1}{2}x$

$$\omega^2 = \frac{c(m_1+m_2)}{m_1m_2}\left[1 \pm \left(1-\frac{1}{2}x\right)\right]$$

$$= \begin{cases} c\frac{(m_1+m_2)}{m_1m_2}\left(2-\frac{1}{2}x\right) \approx 2c\frac{(m_1+m_2)}{m_1m_2} = \omega_1^2 = 2c\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \\ \frac{1}{2}\frac{c(m_1+m_2)}{m_1m_2}x = \frac{c}{2}\frac{k^2a^2}{m_1+m_2} = \omega_2^2 \end{cases}$$

The matrix that we had was

$$\begin{pmatrix}0\\0\end{pmatrix} = \begin{pmatrix} m_1\omega^2 - 2C & C(1+e^{-ika}) \\ C(e^{ika}+1) & m_2\omega^2 - 2C \end{pmatrix}\begin{pmatrix}u\\v\end{pmatrix}$$

In long-wavelength approx. $k \ll 1$ $\quad e^{\pm ika} \approx 1 \pm ika$

$$\begin{pmatrix}0\\0\end{pmatrix} \simeq \begin{pmatrix} m_1\omega^2 - 2C & C(2-ka) \\ C(2+ka) & m_2\omega^2 - 2C \end{pmatrix}\begin{pmatrix}u\\v\end{pmatrix}$$

For $\omega = \omega_1^2 = 2C\left(\frac{1}{m_1}+\frac{1}{m_2}\right)$

$$m_1 2C\left(\frac{1}{m_1}+\frac{1}{m_2}\right)u - 2Cu + C(2-ka)v = 0$$

$$2Cu\frac{m_1}{m_2} + C(2-ka)v = 0$$

$$C(2+ka)u + m_2 2C\left(\frac{1}{m_1}+\frac{1}{m_2}\right)v - 2Cv = 0$$

$$C(2+ka)u + 2C\frac{m_2}{m_1}v = 0$$

At $k=0$

$$2Cu\frac{m_1}{m_2} + 2Cv = 0 \qquad 2Cu + 2C\frac{m_2}{m_1}v = 0$$

$$u\frac{m_1}{m_2} = -v$$

$$\frac{u}{v} = -\frac{m_2}{m_1}$$

Oscillation with oppossite phases

For $\omega^2 = \omega_2^2 = \frac{C}{2}\frac{k^2a^2}{m_1+m_2}$

$$\frac{m_1 C k^2 a^2}{2(m_1+m_2)}u - 2Cu + C(2-ka)v = 0$$

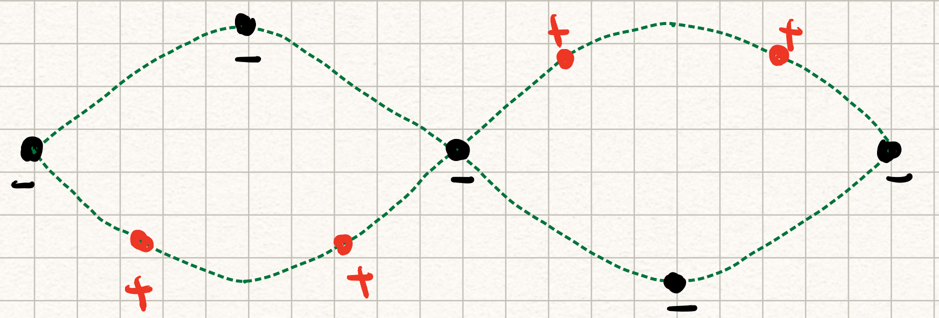
$$c(2+ka)u + \frac{m_2 c k^2 a^2}{2(m_1+m_2)} v - 2cv = 0$$

at $k=0$

$$-2cu + 2cv = 0 \quad \rightarrow \quad u = v$$

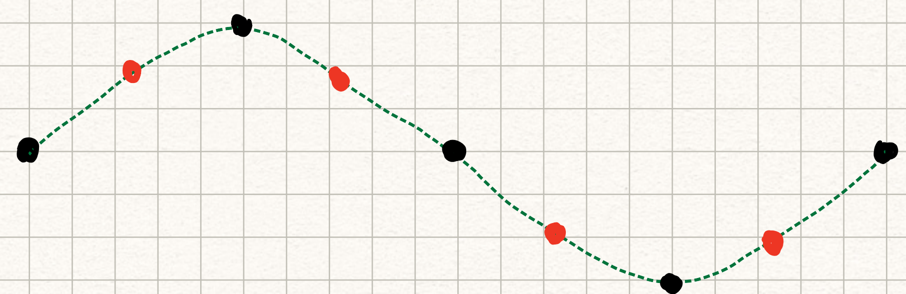
oscillating in phase with the same amplitude

Optical mode: this is how a wave of light would make the charges move

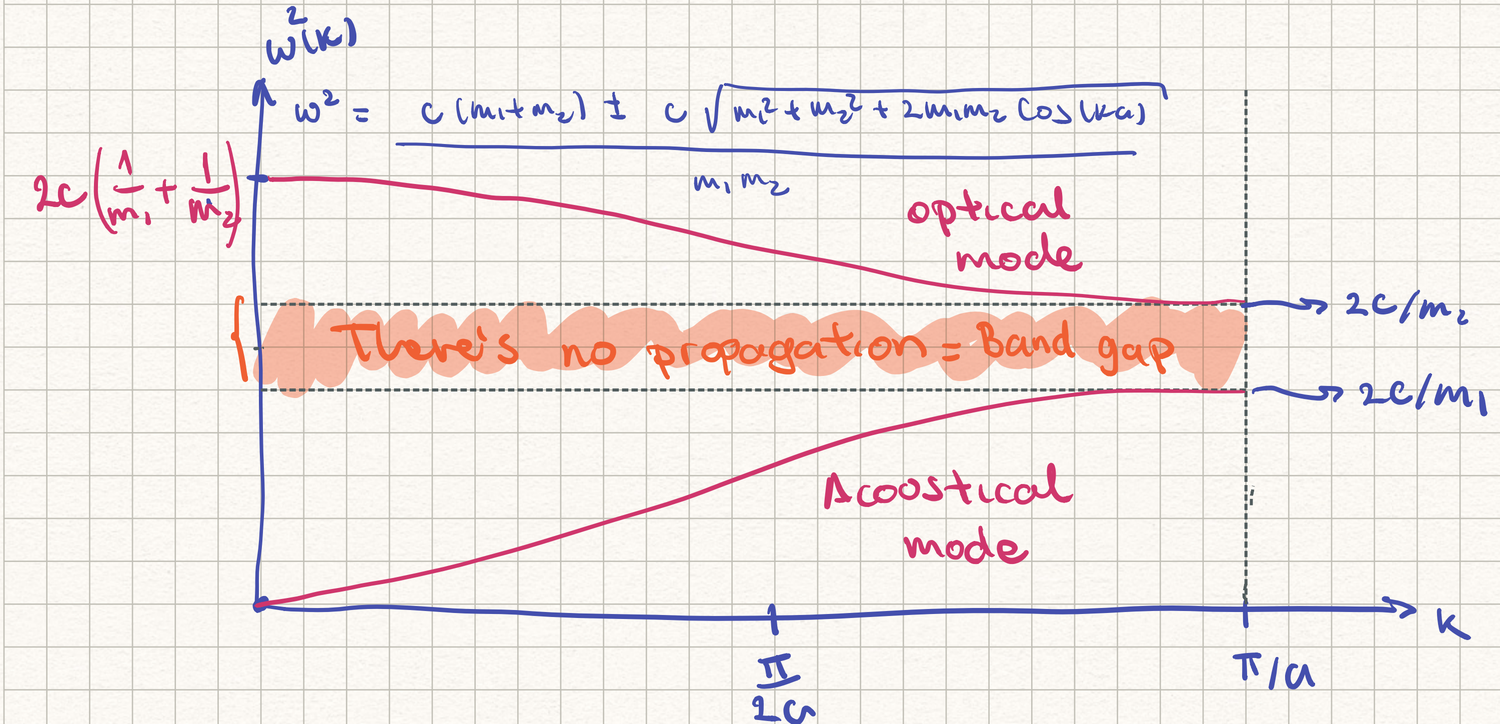


$$\frac{u}{v} = -\frac{m_1}{m_2}$$

Acoustic mode: this how sound propagates



$$\frac{u}{v} = 1$$



$k = \pi/a \qquad \cos(\pi) = -1$

$$\omega^2 = \frac{c\,(m_1+m_2) \pm c\sqrt{m_1^2 + m_2^2 - 2m_1m_2}}{m_1m_2}$$

$$= \frac{c\,(m_1+m_2) \pm c\sqrt{(m_1-m_2)^2}}{m_1m_2} \qquad m_1 > m_2$$

$$= \frac{c\,(m_1+m_2) \pm c\,(m_1-m_2)}{m_1m_2} = \begin{cases} 2c/m_2 \\ 2c/m_1 \end{cases}$$

$k = 0 \qquad \cos(0) = 1$

$$\omega^2 = \frac{c\,(m_1+m_2) \pm c\sqrt{m_1^2 + m_2^2 + 2m_1m_2}}{m_1m_2}$$

$$= \frac{c\,(m_1+m_2) \pm c\sqrt{(m_1+m_2)^2}}{m_1m_2} \qquad m_1 > m_2$$

$$= \frac{c\,(m_1+m_2) \pm c\,(m_1+m_2)}{m_1m_2} = \begin{cases} \frac{2\,(m_1+m_2)c}{m_1m_2} = 2c\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \\ 0 \end{cases}$$

There's a gap in the frequencies

$\frac{2c}{m_1} < \omega^2 < \frac{2c}{m_2}$ There are no wave-like solutions

In polyatomic lattices there's a frequency gap at the boundary of the Brillouin zone $k = \pm\pi/a$

Phonons are the material oscillations of the crystal