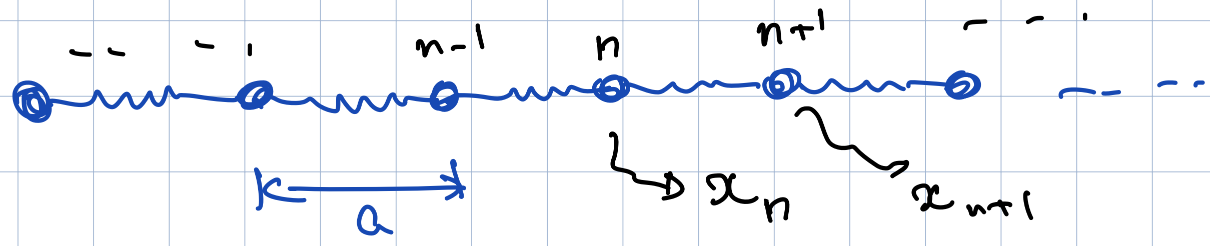
Monatomic Harmonic Chain



low T: quadratic potential holds atoms in place.

$$V_{tot} = \sum_n V(x_{n+1} - x_n)$$

$$= \sum_n \frac{k}{2}(x_{n+1} - x_n - a)^2$$

$$\boxed{x_n = na + \delta x_n}$$

$$= \sum_n \frac{k}{2}(\delta x_{n+1} - \delta x_n)^2$$

$$F_n = -\frac{\partial V_{tot}}{\partial x_n} = m\frac{d^2}{dt^2}(\delta x_n)$$

$$= k(\delta x_{n+1} - \delta x_n) + k(\delta x_{n-1} - \delta x_n)$$

(1) $$m(\ddot{\delta x_n}) = k(\delta x_{n-1} + \delta x_{n+1} - 2\delta x_n)$$

"plane wave ansatz"

(2) $\delta x_n(t) = A\, e^{i\omega t - ik(na)}$

$$-m\omega^2 \cancel{A}\, \cancel{e^{i\omega t}}\, e^{-ikna} =$$

$$K \cancel{A}\, \cancel{e^{i\omega t}} \left[e^{-ik(n-1)a} + e^{-ik(n+1)a} - 2\, e^{-ikna} \right]$$

$$\longrightarrow -m\omega^2 = K \left[e^{ika} + e^{-ika} - 2 \right]$$

$$\longrightarrow \omega^2 = \frac{K}{m} \left[2 - 2\cos ka \right]$$

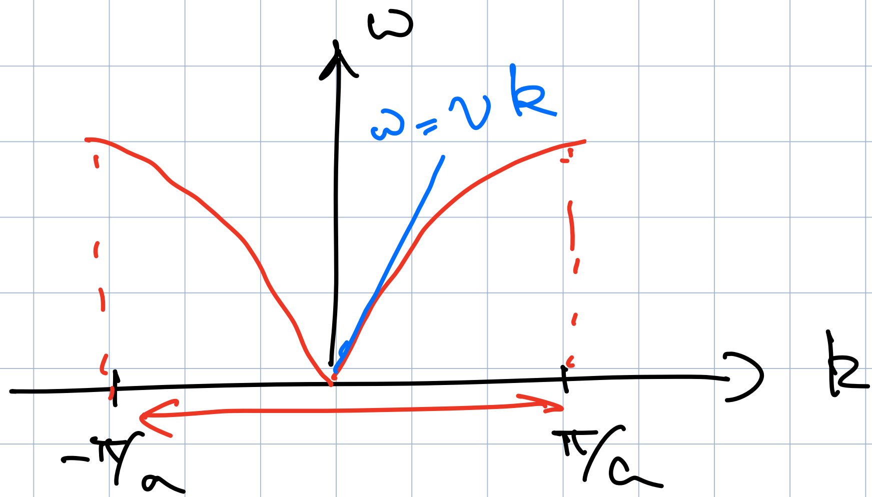
$$= \frac{4K}{m} \sin^2\left(\frac{ka}{2}\right)$$

$$\longrightarrow \omega = 2\sqrt{\frac{K}{m}} \left| \sin \frac{ka}{2} \right|$$

$|k| \ll 1/a$

$$\omega \simeq 2\sqrt{\frac{K}{m}} \left| \frac{ka}{2} \right| = \sqrt{\frac{K}{m}}\, a\, |k|$$

$$\equiv v\, |k|$$



$k \to k + \frac{2\pi}{a}$

1. Sound mode due to low ~~k~~ energy modes
2. The wavevector k is bounded

\# modes in a periodic chain of size $L = Na$

$$e^{ikL} = 1 \quad \longrightarrow \quad k = \frac{2\pi}{L} n$$

$\longrightarrow$ spacing $\Delta k = \frac{2\pi}{L}$

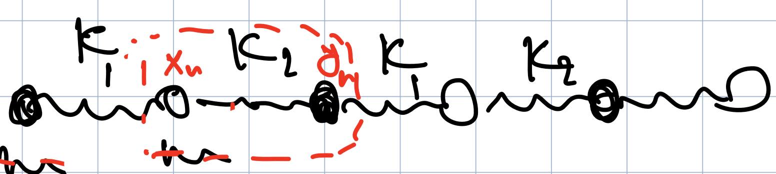
$$\#\text{ modes} = \frac{2\pi/a}{2\pi/L} = \frac{L}{a} = N$$

1D: $$\sum_k \longrightarrow \cancel{\frac{L}{2\pi}\int_{-\infty}^{+\infty} dk} \qquad \frac{L}{2\pi}\int_{-\pi/a}^{\pi/a} dk$$

$$3D: \sum_{\vec{k}} \longrightarrow \left(\frac{L}{2\pi}\right)^3 \int_{-\pi/a}^{\pi/a} dk_x \int_{''}^{''} dk_y \int_{''}^{''} dk_z$$

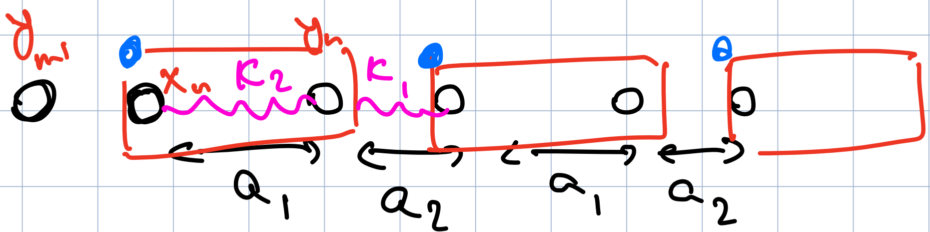
$$\left(\frac{L}{2\pi}\right)^3 \downarrow \frac{V}{(2\pi)^3}$$

Diatomic system



$\circ = x_n,\ \delta x_n$

$\bullet = y_n,\ \delta y_n$



$$m\,\delta\ddot{x}_n = k_2(\delta y_n - \delta x_n) + k_1(\delta y_{n-1} - \delta x_n)$$

$$m\,\delta\ddot{y}_n = k_1(\delta x_{n+1} - \delta y_n) + k_2(\delta x_n - \delta y_n)$$

$$\delta x_n = A_x\, e^{i\omega t - ikna}$$

$$\delta y_n = A_y\, e^{i\omega t - ikna}$$

$$-m\omega^2 A_x\, \cancel{e^{i\omega t}}\, e^{-ik\boxed{n}a} = k_2 A_y\, \cancel{e^{i\omega t}}\, e^{-ik\boxed{n}a} + k_1 A_y\, \cancel{e^{i\omega t}}\, e^{-ik(\boxed{n}-1)a} - (k_1+k_2) A_x\, \cancel{e^{i\omega t}}\, e^{-ik\boxed{n}a}$$

$$-m\omega^2 A_y\, e^{i\omega t - ikna} = k_1 A_x\, e^{i\omega t - ik(n+1)a} + k_2 A_x\, e^{i\omega t - ikna} - (k_1+k_2) A_y\, e^{i\omega t - ikna}$$

$$\begin{cases} -m\omega^2 A_x = -(K_1+K_2)A_x + (K_2+K_1e^{ika})A_y \\ -m\omega^2 A_y = (K_2+K_1e^{-ika})A_x - (K_1+K_2)A_y \end{cases}$$

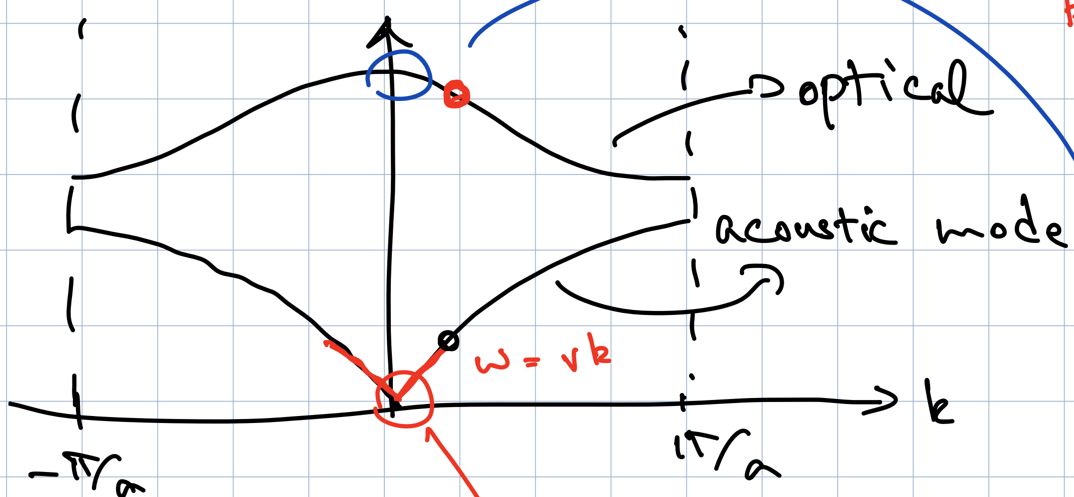
$$\rightsquigarrow \quad -m\omega^2 \begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{pmatrix} -(K_1+K_2) & K_2+K_1e^{ika} \\ K_2+K_1e^{-ika} & -(K_1+K_2) \end{pmatrix} \begin{pmatrix} A_x \\ A_y \end{pmatrix}$$

eigenvalue problem

$$m\omega^2 = K_1+K_2 \pm \left| K_2+K_1e^{ika} \right|$$

For each k, two solutions for ω

$k_{light} = \frac{\omega}{c}$



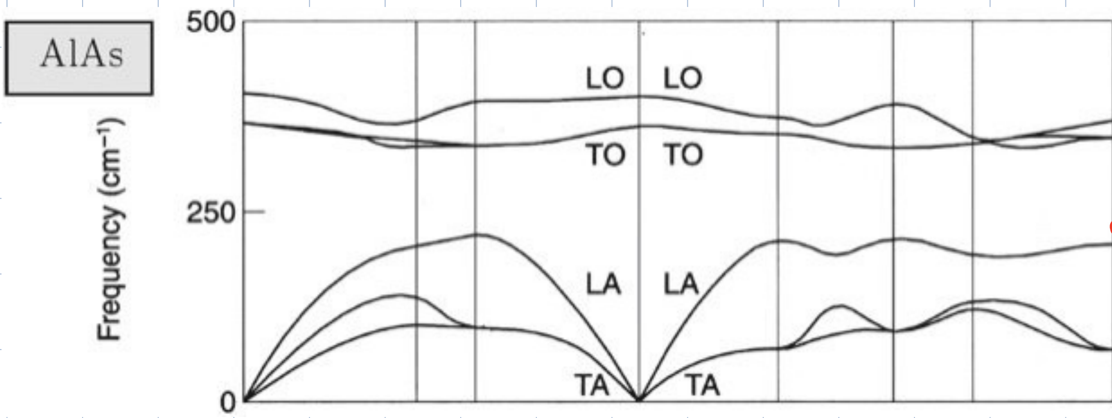
$$k \to 0 \quad \begin{cases} \to \omega = 0 \\ \to \omega = \sqrt{\dfrac{2(K_1+K_2)}{m}} \end{cases}$$

If M atoms in unit cell.

at each k, M different branches

1 acoustic

$M-1$ optical



optical

acoustic