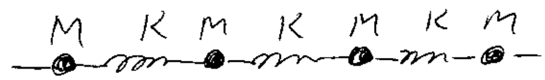
Phys 617   Oct. 9, 2007

Lattice Vibrations –



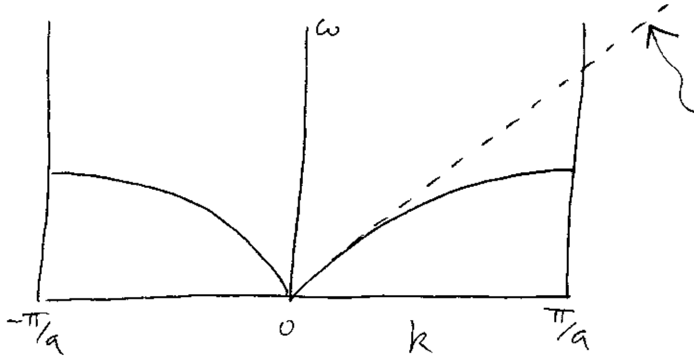
simple 1D case,
$K \simeq$ simple spring $F = -Kx$

classical eqn. of motion $\Rightarrow$ $M\ddot{u}_i = K(u_{i+1} - 2u_i + u_{i-1})$

- solution is $u = u_0 e^{i(kx - \omega t)}$
- also assume periodic boundary conditions $\Rightarrow$ $k = \left(\frac{2\pi}{L}\right)\cdot m$

- plug in to above yields,

$$\omega^2 = \frac{4K}{M}\sin^2\left(\frac{ka}{2}\right) \rightarrow \boxed{\omega = 2\sqrt{\frac{K}{M}}\left|\sin\frac{ka}{2}\right|}$$

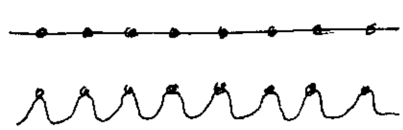


line is solution for elastic continuum, where $\omega = \sqrt{\frac{Ka^2}{M}}\,k$,

and $\sqrt{\frac{Ka^2}{M}}$ = speed of sound,

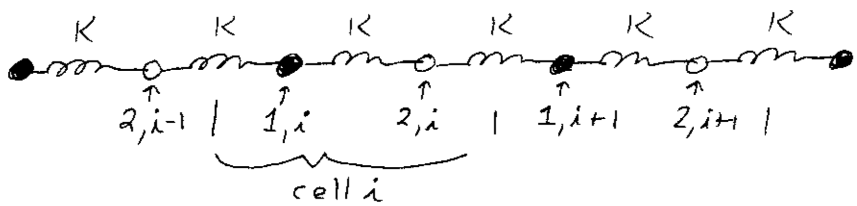
Note: we can limit ourselves to k inside 1st Brillouin zone, since sol'ns $\left(k \pm \frac{2\pi}{a}\right)$ are same as soln. k:

e.g.



$\left.\begin{array}{l} k=0 \\ k=\frac{2\pi}{a} \end{array}\right\}$ same thing (u measured only at discrete points.)

Simple example, basis of 2 atoms



$\bullet = M$

$\circ = M'$

eqns. of motion

$$M\ddot{u}_{i1} = K\,(u_{i2} - 2u_{i1} + u_{i-1,2})$$

$$M'\ddot{u}_{i2} = K\,(u_{i1} - 2u_{i2} + u_{i+1,1})$$

has a soln,

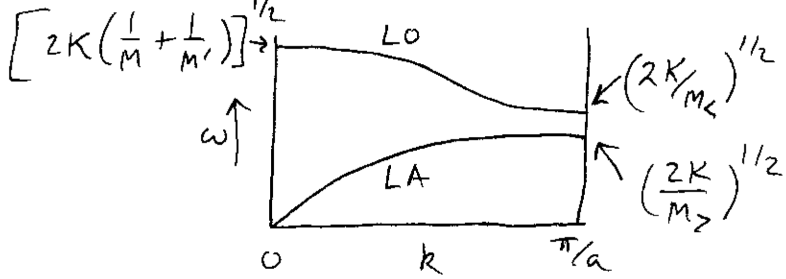
$$u_{i(1,2)} = \epsilon_{1,2}\, e^{i(kx_i - \omega t)}$$

gives,

$$\begin{bmatrix} \omega^2 - 2K/M & \frac{K}{M}(1+e^{-ika}) \\ \frac{K}{M'}(1+e^{ika}) & \omega^2 - 2K/M' \end{bmatrix} \cdot \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \end{pmatrix} = 0$$

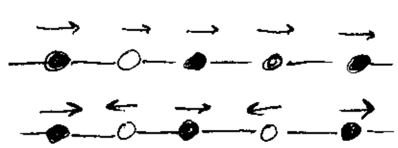
solve ...

$$\omega^2 = \frac{K(M+M')}{MM'}\left[1 \pm \sqrt{1 - \frac{2MM'}{(M+M')^2}(1-\cos ka)}\right]$$



has 2 branches

at $k=0$:



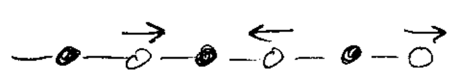
"Acoustic"

$\omega = 0$ soln $\epsilon_1 = \epsilon_2$

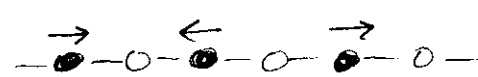
upper soln $\epsilon_1 = -\epsilon_2$

"optical

at $k = \frac{\pi}{a}$



$\omega^2 = \frac{2K}{M'}$, $\begin{cases} \epsilon_1 = 0 \\ \epsilon_2 = \text{any} \end{cases}$



$\omega^2 = \frac{2K}{M}$

$\hookrightarrow \epsilon_2 = 0$