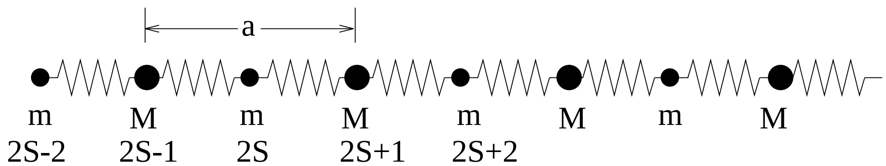
Physics 0551 Lecture #11

A one dimensional chain with a two "mass" basis

So far we have discussed the simplest situation possible, a linear chain with one atom per basis. We can complicate the situation by either changing the Spring constants **or** altering the masses along the chain. We will alter the masses.



Even numbered atoms have mass m

Odd numbered atoms have mass M

$$\begin{aligned} F_{2s} &= m\,\ddot{u}_{2s} = c[u_{2s+1} + u_{2s-1} - 2u_{2s}] \\ F_{2s+1} &= M\,\ddot{u}_{2s+1} = c[u_{2s+2} + u_{2s} - 2u_{2s+1}] \end{aligned}$$

Assume wave solutions

$$\longleftarrow \quad u_{2s} = E\ e^{i(2sk\,a/2)}\exp^{-i\omega t};\ u_{2s+1} = Oe^{i((2s+1)ka/2)}\exp^{-i\omega t}$$

$$\longleftarrow \quad \ddot{u}_{2s} = -E\omega^2 e^{i(2sk\,a/2)} exp^{-i\omega t};\ \ddot{u}_{2s+1} = -O\omega^2 e^{i((2s+1)k\,a/2)} exp^{-i\omega t}$$

Substitute:

$$\longrightarrow \quad -m\omega^2 E e^{i2sk\,a/2} = c[Oe^{i(2s+1)k\,a/2} + Oe^{i(2s-1)ka/2} - 2Ee^{i2sk\,a/2}]$$

$$-m\omega^2 E = c[Oe^{ika/2} + Oe^{-ika/2} - 2E]$$

and

$$-M\omega^2 O = c[Ee^{ik\,a/2} + \mathrm{E}\ e^{-ik\,a/2} - 2O]$$

$$\boxed{(2c - m\omega^2)E - (2c\ \cos(ka/2))O = 0} \ \mathbf{A}$$

$$\boxed{(2c - M\omega^2)O - (2c\ \cos(ka/2))E = 0} \ \mathbf{B}$$

Rearranging B

$-(2c\cos ka/2)E - (2c - M\omega^2)\ \mathrm{O} = 0$

These two equations have solutions if $|\det| = 0$. (Hence solutions are coupled)

$$\left| \begin{bmatrix} 2c - m\omega^2 & -2c\cos\ ka/2 \\ & \\ -2c\ \cos\ ka/2 & 2c - M\omega^2 \end{bmatrix} \right| = 0$$

$$4c^2 - 2c(m+M)\omega^2 + Mm\omega^4 - 4c^2\cos^2 ka/2 = 0$$

$$\omega^2 = \frac{2c(m+M) \pm \sqrt{4c^2(m+M)^2 - 4Mmc^2 - 4c^2\cos^2 ka/2)}}{2Mm}$$

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

Note we have *two* solutions.
Examine limiting cases:

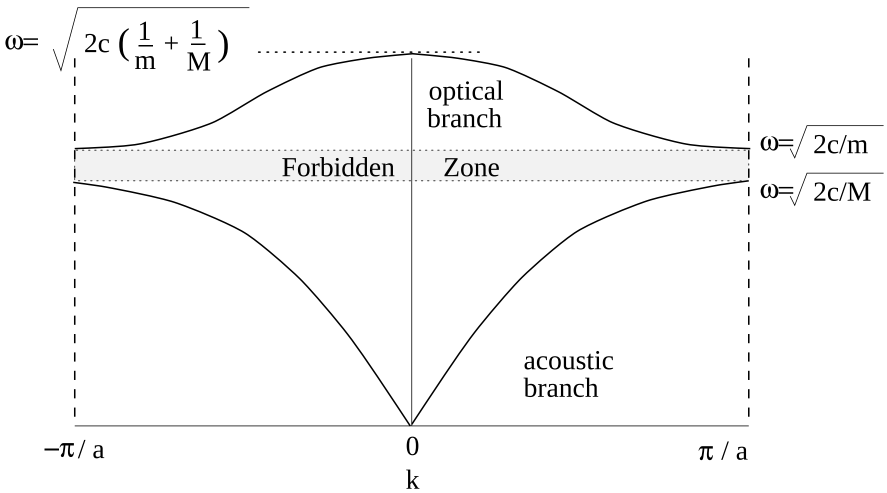
$$\begin{array}{lll} k = 0 & \omega^2 = 0 & - \\ & \omega^2 = 2c\left(\frac{1}{M} + \frac{1}{m}\right) & + \\ k = \frac{\pi}{a} & \omega^2 = 2c\left(\frac{1}{M} + \frac{1}{m}\right) \pm 2c|\left(\frac{1}{m} - \frac{1}{M}\right)|;\ (\sin\frac{\pi}{2} = 1) & \end{array}$$

since $m < M$ and $\frac{1}{m} > \frac{1}{M}$

$\omega^2 = \frac{2c}{m}$ for $+$

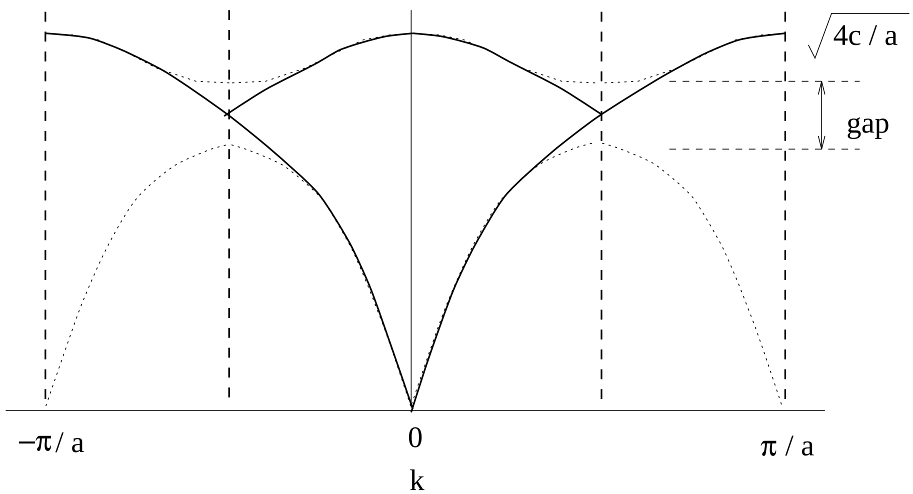
$\omega^2 = \frac{2c}{M}$ for $-$

Now to plot the dispersion curves



Notice the *gap* in frequencies.

The oscillations in this gap cannot be supported. How can we think about this in direct comparison with the previous model. (The single mass chain)

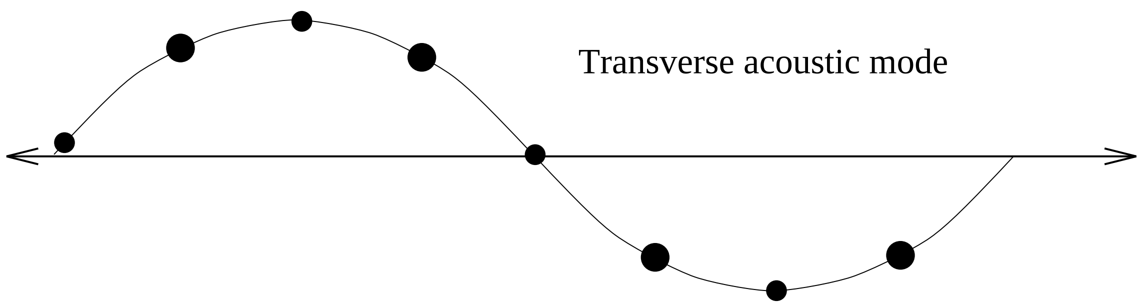


What do these modes look like

At $k = 0$ for the acoustic branch, the atoms vibrate in phase.

$$(2c - \omega^2 m)E - (2c\ \cos ka/2)O = 0$$

$$E - O = 0 \text{ or } E = O$$



At $k = 0$ for the optical branch (+ sign)

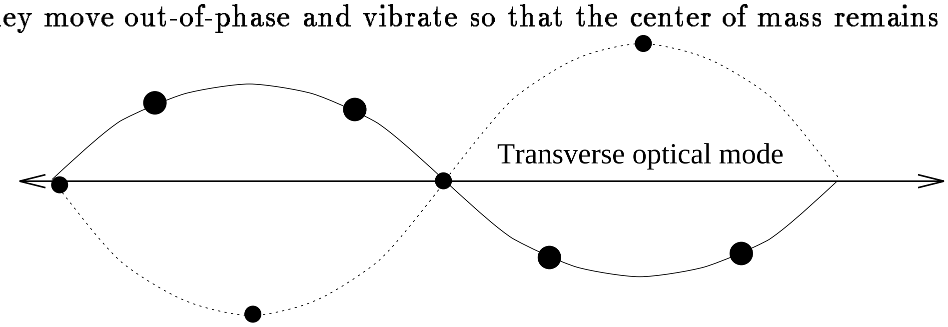
$$\omega^2 = 2c\left(\frac{1}{m} + \frac{1}{M}\right)$$

$$\left(2c - 2m\left(\frac{1}{m} + \frac{1}{M}\right)\right)E - 2cO = 0$$

$$-\frac{m}{M}E = O$$

$$-mE = MO$$

They move out-of-phase and vibrate so that the center of mass remains constant.



If we have an ionic crystal, m and M may have different electronic charge. Hence there are moving dipoles which can absorb or emit light (optical modes). Note that we can have only **vertical** transitions since the given infrared photons have no momentum of any significance !

This process is called Restsrahlen (residual)