Note on lattice vibrations of a linear chain with 2 atoms:

Point 1: Derivation of dispersion relation.

In the lecture following two couple equations were derived from a linear chain with two different atoms with mass M_1 and M_2.

$$\begin{bmatrix} \omega^2 M_1 - 2C & C(1+e^{ika}) \\ C(1+e^{-ika}) & \omega^2 M_2 - 2C \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

The couple equations have a solution when the determinant is zero. Remember that det(A) =ab-cd when A=$\begin{bmatrix} a & d \\ c & b \end{bmatrix}$. We have wish to solve

$$\det\begin{bmatrix} \omega^2 M_1 - 2C & C(1+e^{ika}) \\ C(1+e^{-ika}) & \omega^2 M_2 - 2C \end{bmatrix} = M_1 M_2 \omega^4 - 2C(M_1+M_2)\omega^2 + 2C^2[1-\cos(ka)] = 0$$

Lets now change variable: $\alpha = \omega^2$and $\widetilde{M} = \frac{M_1 M_2}{M_1+M_2}$.

Our equation now simplifies to:

$$\alpha^2 - \frac{2C}{\widetilde{M}}\alpha + \frac{2C^2}{M_1 M_2}[1-\cos(ka)] = 0$$

This is a second order equation of the form $x^2 - bx + c = 0$ where a,b and c are constants. The solution is then x=$\frac{b \pm \sqrt{b^2-4c}}{2}$. The dispersion relation thus read:

$$\omega^2 = \alpha = \frac{C}{\widetilde{M}}\{1 \pm \sqrt{1 - \frac{2\widetilde{M}}{M_1 M_2}[1-\cos(ka)]}\}$$

Notice that there are actually two solutions as depicted in the figure below.

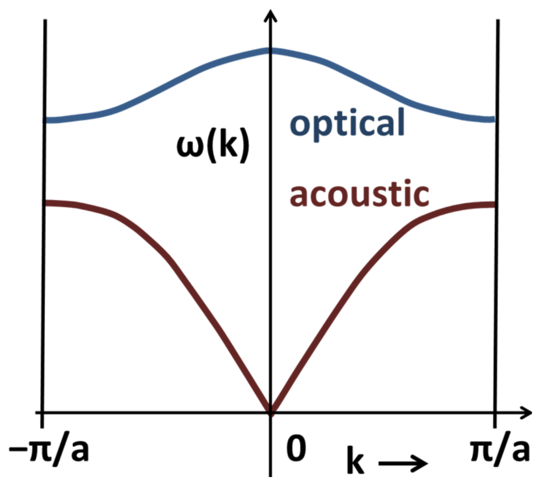

Figure 1 is taken from: https://en.wikipedia.org/wiki/Phonon

It shows the two dispersion of the above derived equation.

Point 2: Inspection of the vibration amplitudes in the long wave length limit: ka → $\mathbf{0}$.

Use the following two Taylor expansions: $\cos(x) \approx 1 - 0.5x^2$ and $\sqrt{1+x} = 1 + 0.5x$ to derive:

$$\omega^2 = \alpha = \frac{C}{\tilde{M}}\{1 \pm (1 - \frac{\tilde{M}k^2a^2}{M_1M_2})\} = \begin{cases} 2C\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \\ \frac{Ck^2a^2}{2(M_1+M_2)} \end{cases}$$

The blue solution is coming from the plus option whereas the red solution is originating from the minus option. Notice also the the "blue" solution correspond to the "optical" branch shown in Figure 1 and the "red" solution correspond to the "acoustic" branch.

Our original equations read: $[\omega^2 M_1 - 2C]x + [C(1 + e^{ika})]$y = 0. We can now inspect the two amplitudes (x and y) for the optical and acoustic branch in the ka → 0 limit.

Vibration amplitudes for the optical branch ("blue" solution)

In the limit we are considering this simplifies to $[\omega^2 M_1 - 2C]x + 2Cy = 0$. Now we can insert ω^2 solutions. Let's start with the blue solution.

$$[\omega^2 M_1 - 2C]x + 2Cy = [2CM_1\left(\frac{1}{M_1} + \frac{1}{M_2}\right) - 2C]x + 2Cy = 0$$

This simplifies to $\frac{x}{y} = -\frac{M_2}{M_1}$. The important meaning of this is that the amplitudes x and y have opposite signs. The two atoms are therefore moving in opposite directions.

Vibration amplitudes for the acoustic branch ("red" solution)

Let's now look at the "red" solution.

$$[\omega^2 M_1 - 2C]x + 2Cy = [M_1 \frac{Ck^2a^2}{2(M_1+M_2)} - 2C]x + 2Cy = 0$$

In the limit ka → 0 we have x=y meaning that the amplitudes have the same sign and hence the two atoms are moving in the same direction.