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.

\[
\begin{align*}
\bullet & \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \\
& \quad m \quad M \quad m \quad M \quad m \quad M \quad m \quad M \\
2S-2 & \quad 2S-1 \quad 2S \quad 2S+1 \quad 2S+2
\end{align*}
\]

Even numbered atoms have mass \( m \)

Odd numbered atoms have mass \( M \)

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

Assume wave solutions

\[
\begin{align*}
\longleftrightarrow u_{2s} &= E e^{i(2sk \alpha/2)} \exp^{-i\omega t}, \quad u_{2s+1} = O e^{i((2s+1)k\alpha/2)} \exp^{-i\omega t} \\
\longleftrightarrow \ddot{u}_{2s} &= -E\omega^2 e^{i(2sk \alpha/2)} \exp^{-i\omega t}, \quad \ddot{u}_{2s+1} = -O\omega^2 e^{i((2s+1)k\alpha/2)} \exp^{-i\omega t}
\end{align*}
\]

Substitute:

\[
\begin{align*}
\longrightarrow -m\omega^2 E e^{i2sk \alpha/2} &= c[Oe^{i(2s+1)k\alpha/2} + Oe^{i(2s-1)k\alpha/2} - 2Ee^{i2sk \alpha/2}] \\
-m\omega^2 E &= c[Oe^{ik\alpha/2} + Oe^{-ik\alpha/2} - 2E]
\end{align*}
\]

and

\[
-M\omega^2 O = c[Ee^{ik\alpha/2} + E e^{-ik\alpha/2} - 2O]
\]

\[
\begin{align*}
\frac{(2c - m\omega^2)E - (2c \cos (ka/2))O}{(2c - M\omega^2)O - (2c \cos (ka/2))E} &= 0 \\
A & \quad B
\end{align*}
\]

Rearranging B

\[-(2c \cos (ka/2))E - (2c - M\omega^2) O = 0 \]
These two equations have solutions if $|\text{det}| = 0$. (Hence solutions are coupled)

\[
\begin{bmatrix}
2c - m\omega^2 & -2c \cos \frac{ka}{2} \\
-2c \cos \frac{ka}{2} & 2c - M\omega^2
\end{bmatrix} = 0
\]

\[4c^2 - 2c(m + M)\omega^2 + Mm\omega^4 - 4c^2 \cos^2 \frac{ka}{2} = 0\]

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

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

Note we have two solutions.

Examine limiting cases:

\[
k = 0 \quad \omega^2 = 0 \\
k = \frac{\pi}{a} \quad \omega^2 = 2c \left( \frac{1}{M} + \frac{1}{m} \right) \pm 2c \left| \left( \frac{1}{m} - \frac{1}{M} \right) \right|; \ (\sin \frac{\pi}{2} = 1)
\]

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

\[
\omega^2 = \frac{2c}{m} \text{ for } +
\]

\[
\omega^2 = \frac{2c}{M} \text{ for } -
\]

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 \textbf{vertical} transitions since the given infrared photons have no momentum of any significance!

This process is called Reststrahlen (residual)