Phonons

1D monatomic chain: let's start with a 1 dimensional crystal lattice with mass M. When we talked about the harmonic oscillator, we showed that the atomic potential can be approximated by a quadratic form near the minimum (near the equilibrium position). This is equivalent to a string of masses with springs having a spring constant \( K \) between them.

\[
\begin{align*}
\text{Atom} & \quad \text{new equilibrium position} \\
X_j & \quad \text{and displacement} = a \text{ current} + \delta_u_j = x_j - x_j
\end{align*}
\]

Force \( F_j \) acting on atom \( j \) is the sum of forces from the neighbors.

\[
F_j = K (u_{j+1} - u_j) - K (u_j - u_{j-1})
\]
Let us use the classical approach where $F = ma$ so that

$$m \frac{d^2 u_j}{dt^2} = k(u_{j+1} - u_j) - k(u_j - u_{j-1})$$

This is a wave equation for displacement and it is solved by a wave

$$u_j = A \exp \left[ -i(\omega t - kx) \right]$$

Substituting this solution gives

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

Solve for $\omega_k$ as

$$u(k) = 2 \sqrt{\frac{k}{m}} \left| \sin \left( \frac{ka}{2} \right) \right|$$

![Graph of $u(k)$ with values at $\frac{2\pi}{a}$, $\frac{4\pi}{a}$, $\frac{6\pi}{a}$, and $\frac{8\pi}{a}$]
\[ E = \hbar w(k) \text{ again periodic in } k \]
and all the information we need about \( E = \hbar w(k) \) is contained in the range \(-\pi/a < k < \pi/a\) which is the 1st Brillouin zone in 1D.

Applying the Born-von Karman BC that \( u(0) = u(Na) \) gives us allowed wavevectors \( k = \frac{2\pi n}{Na} \) \((n = 0, \pm 1, \pm 2, \ldots)\).

For \( k = 2\pi/\lambda \) where \( \lambda \) is the wavelength, we note that if \( N > N/2 \), then \( \lambda < 2a \) which would mean there are no atoms between 1 period. This, of course, is meaningless since we cannot talk about displacement & when there are no atoms present:

\[
\lambda = \frac{4a}{5} \quad \text{or} \quad \frac{10\pi}{4a} = 2 \frac{1}{2} \frac{11}{a}
\]

\[ k = 2\pi/\lambda = \frac{\pi}{a} \quad \text{or} \quad k = 2\pi/\lambda = \frac{10\pi}{4a} = 2 \frac{1}{2} \frac{11}{a} \]
Phase vs. Group Velocity

\[ V_p = \frac{\omega}{k} \] is the phase velocity at which a single wave propagates.

\[ w = A \exp \left[ i \left( \omega t - kx \right) \right] \Rightarrow \omega t - kx = \text{const}. \]

Now consider a simple wave packet made up of two harmonic waves:

\[ \psi = \sin \left( k_1 x - \omega_1 t \right) + \sin \left( k_2 x - \omega_2 t \right) \]

This wave packet can be expressed as:

\[ \psi = 2 \sin \left( k_0 x - \omega_0 t \right) \cos \left( \Delta k x - \Delta \omega t \right) \]

where \( k_0 = \frac{k_1 + k_2}{2} \) and \( \omega_0 = \frac{\omega_1 + \omega_2}{2} \)
and \( \Delta k = \frac{k_2 - k_1}{2} \), \( \Delta \omega = \frac{\omega_2 - \omega_1}{2} \)

The modulation pattern (the \( \cos(\Delta k x - \Delta \omega t) \)) moves at a speed where

\[ \Delta k x - \Delta \omega t = \text{const}. \]

Differentiating with time gives

\[ v_g = \frac{dx}{dt} = \frac{\Delta \omega}{\Delta k} \]
In the limit of small \( \Delta w \) and \( \Delta k \) (highly localized wave packet) we can write
\[
v_g = \frac{d \omega(k)}{dk}
\]
or in 3D \[
v_g = 7k a \omega(E)
\]

In our 1D example we obtain a group velocity of
\[
v_g = \frac{d \omega}{dk} = J \frac{K a^2}{m} \cos \frac{1}{2} k a
\]

At the edge of the 1st BZ \( k = \pi/a \) and \( v_g = 0 \). This means at the edge of the BZ, where \( \lambda = 2a \) we have a standing wave
\[
u_j = A \exp \left[-i(\omega t - k_j x)\right] = A \exp \left[-i(\omega t - \pi x)\right]
\]

A standing wave carries no energy even though the phonon velocity is
Still \( \omega (m/a) = 2 \sqrt{\frac{K}{m}} \) \( V_p = \frac{\omega}{K} = \frac{2\alpha}{\pi} \sqrt{\frac{E}{m}} > 0 \)

**Diatomic chain:** we have two different masses \( m_1 \) and \( m_2 \)

so we have 2 atoms per basis.

We look for solutions to the 2 displacement \( U_j \) and \( V_j \) of the 2 masses

\[
\begin{align*}
m_1 \frac{d^2 U_j}{dt^2} & = K (V_j + V_{j-1} - 2U_j) \\
m_2 \frac{d^2 V_j}{dt^2} & = K (U_{j+1} + U_j - 2V_j)
\end{align*}
\]

Solutions are two traveling waves

\[
\begin{align*}
U_j & = A \exp \left[-i (\omega t - jka)\right] \\
V_j & = A \exp \left[-i (\omega t - jka)\right]
\end{align*}
\]

Substituting we get

\[
\begin{align*}
-\omega^2 m_1 U_j & = KV_j (1 + e^{ika}) - 2KU_j \\
-\omega^2 m_2 V_j & = KU_j (e^{-ika} + 1) - 2KV_j
\end{align*}
\]
Again we can solve the system using the determinant

\[
\begin{vmatrix}
2K - m_1 \omega^2 & -K(1 + e^{i\kappa a}) \\
-K(1 + e^{i\kappa a}) & 2K - m_2 \omega^2
\end{vmatrix} = 0
\]

or

\[
m_1 m_2 \omega^4 - 2K(m_1 + m_2) \omega^2 + 2K^2 (1 - \cos \kappa a) = 0
\]

Thus

\[
\omega^2 = \frac{K \left( m_1 + m_2 \pm \sqrt{m_1^2 + m_2^2 + 2m_1 m_2 \cos \kappa a} \right)}{m_1 m_2}
\]

Special case \( m_1 = m_2 = m \)

\[
\omega^2 = \frac{K}{m} \left( 2 \pm \sqrt{2 + 2 \cos \kappa a} \right)
\]

The graph shows the first Brillouin zone (BZ) with special points labeled.
- Other special cases: small \( k a \)
  
  \[
  \cos (k a) \approx 1 - \frac{1}{2} k^2 a^2 + O(k^4 a^4)
  \]

  \[
  \omega^2 \approx 2K \left( \frac{1}{m_1} + \frac{1}{m_2} \right) \quad \text{optical}
  \]

  \[
  \omega^2 \approx \frac{k}{\frac{1}{m_1} + \frac{1}{m_2}} (k a)^2 \quad \text{acoustic}
  \]

  Note that the acoustic dispersion is linear in \( k \) while optical is constant because \( \lambda(k) / \nu(k) = -\frac{m_1}{m_2} \)

  - At \( k = \frac{\pi}{a} \) we have

  \[
  \omega^2 = 2K/m_1 \quad \text{and} \quad 2k^2/m_2
  \]

  If \( m_1 \neq m_2 \) we have a gap between acoustic and optical phonon branches.

\[
\begin{align*}
\omega & \quad \text{versus} \quad k
\end{align*}
\]
What about real crystals in 3D:

In 3D we have 3 degrees of freedom per atom so we get 3 acoustic branches: 1 longitudinal and 2 transverse.

![Diagram of acoustic branches with labels Ti, T1, T2]

If we have n atoms per basis, we still keep the 3 acoustic branches, but now have 3n branches in total. The remaining 3(n-1) are all optical.

Ex. Silicon has 3 acoustic and 3 optical branches.