Summary: We begin these notes by finding a way to solve for allowed phonon modes in a finite crystal. We then give a couple of examples of this calculation. Next we introduce the density of states as a way to count the number of phonon modes per unit volume and solve for an expression for the density of states for both a 9 atom chain and a 1 cm long sample.

- **Goal 1:** Consider which phonon modes within the first Brillouin zone are *allowed* due to finite crystal effects
- Continue to assume that our solid has no surface: If we take our 1D chain of atoms, interatomic spacing \( a \) and total length \( L \), and bend it into a ring we have no exposed surfaces!
- We have a traveling wave solution, \( u_n \)
  - Due to periodic boundary conditions \( u_n = u_{n+N} = u_{n+2N} \ldots \) where \( N \) is the total number of cells in our chain
- Since \( u_n = u_{n+N} e^{i(qx_N + \omega t)} = e^{i(qx_{n+N} + \omega t)} \)
  - Let \( x = na \) and \( x_{n+N} = (n+N)a \)
  - Dividing out the \( e^{i\omega t} \) term we are left with \( 1 = e^{iNa} \)
  - For this to be true: \( q = \frac{2\pi}{Na} n_i \) where \( n_i \) is an integer
- \( n_i \) determines how many modes we have in the crystal
- Since \( q \) is bounded by \( -\frac{\pi}{a} \) to \( \frac{\pi}{a} \) for unique solutions (Nyquist argument concerning the first Brillouin zone), using our \( q = \frac{2\pi}{Na} n_i \) equation, \( n_i \) is bounded from \( -\frac{N}{2} \) to \( \frac{N}{2} \)
- Since \( n_i \) is an integer the number of unique modes is equal to the number of cells in our 1D crystal: \( N \)
- **Conclusion:** Now we know that vibrational modes are discrete in \( q \), bounded by the first brillouin zone and a finite solid has a finite number of unique modes \( q \)

**Example 1:** Chain of 5 atoms
- \( n_i \) ranges from \( -\frac{N}{2} \) to \( \frac{N}{2} \), thus \( -2.5 \leq n_i \leq 2.5 \)
• As an integer, \( n_i = -2, -1, 0, 1, 2 \) for 5 total modes
  
  o Brillouin zone bounds? Brillouin zone boundary at \( q = \frac{\pi}{a} \).
  
  ▪ Since \( a = \frac{L}{N} \), \( \frac{\pi}{a} = \frac{N\pi}{L} \)
  
  ▪ Recall allowed \( q \) occur at \( q = \frac{2\pi}{N a} n_i = \frac{2\pi}{L} n_i \)

Resulting \( q \) space

Example 2: Expanding out to a 1 cm long sample
  
  o Spacing between modes shrinks a lot, since \( L \) is much larger
  
  o Brillouin zone stays the same (\( a \) unchanged) so there are a lot more modes in this sample
  
  o Let \( a=10^{-9} \) m and \( L=10^{-2} \) m

  o \( N = \frac{L}{a} \) so \( 10^7 \) modes in this sample

• Although we drew the dispersion as a line it is actually made up of a \textit{discrete} set of points
  
  o So close together they basically form a line

Density of states

• Phonon dispersion can provide insight into material properties; however, the phonon dispersion is a non-trivial function in 3D and it is often helpful to bin modes by energy to simplify the description of what modes are present in a solid.

• The density of states is the number of modes within a \( E \) to \( E+dE \) per unit volume (depending on the book, some people skip the “per unit volume part”)

• Example: 1D chain of 9 atoms
Dispersion is in terms of $\omega$, we want energy but this is just $\hbar \omega$ for our harmonic oscillator so to simplify just leave in terms of $\omega$ for one less variable. 

Above is the binning of energy levels

Now plot number of states versus omega

More modes at higher energies

Modes are not the same thing as phonons!

**Concept check:** Density of states describes how many vibrational modes are at a particular level, *not* the amplitude (phonon population) of these modes. Each mode’s amplitude will depend on the temperature of the solid.

Now extend to 1 cm sample (finite, but very dense q-spacing)

Ultimately want the number of modes in a given dq and d$\omega$

In 1D, the number of modes in a window dq is just the spacing of the modes times dq

We can multiply by two to count both positive and negative values: $\frac{L}{\pi} dq$
Density of states = \( D(\omega) \)

Invoke an equality: \( D(\omega) \, d\omega = \frac{L}{\pi} \, dq \)

**Talking through equation:** We determine the total number of modes within a window \( d\omega \) about frequency \( \omega \) by taking the product of the density of states at a particular frequency omega with the size of the window. This invokes that \( D(\omega) \) does not change significantly within \( d\omega \), aka that \( d\omega \) is small. Now things get a little tricky. There must exist a \( dq \) that leads to the same number of modes on the right side. We showed above that \( \frac{L}{\pi} \, dq \) will give us the number of modes within a \( dq \). Note that due to the regular spacing of \( q \) points along the \( q \) axis, it doesn’t matter which \( q \) we’re at, just the size of the window \( dq \). Now we manipulate this *equality* to put it into a useful form:

- now multiply by \( d\omega/d\omega \)
- \( D(\omega) \, d\omega = \frac{L}{\pi} \, dq \left( \frac{d\omega}{d\omega} \right) = \frac{L}{\pi} \left( \frac{d\omega}{dq} \right) = \frac{L}{\pi} \left( \frac{d\omega}{v_g} \right) \) Group velocity \( v_g \)!

Recall \( v_g = \sqrt{\frac{c}{m}} \cos\left(\frac{qa}{2}\right) \) for a 1D chain of atoms with a one-atom basis. Plug it in to expression above.

Trouble: We want \( D(\omega) \) in terms of \( \omega \), not \( q \).

Solve \( \omega = \sqrt{\frac{4c}{m}} \sin\left(\frac{qa}{2}\right) \) for \( q \) and plug this back in to \( v_g \)

*Mathematica to the rescue* \( D(\omega) \, d\omega = \frac{L}{\pi} \, dq \sqrt{\frac{c}{m}} \frac{\omega^2}{4} \)

Plot \( D \) versus omega
• Density of states explodes near the edge of the first brillouin zone because the slope of the dispersion (aka group velocity) approached 0 here
• There is an inverse relationship between $v_g$ and the density of states; when you look at an experimental DOS and see a region of spiking DOS, you know the associated dispersion must have a flat region at that energy.
Questions to Ponder

1. How will the density of states be different if we look at a 2D or 3D solid?

2. How will a 2 atom basis change the density of states, if it does at all?