

Topic 5-4: Phonon Density of States
Kittel Pages: 109,110

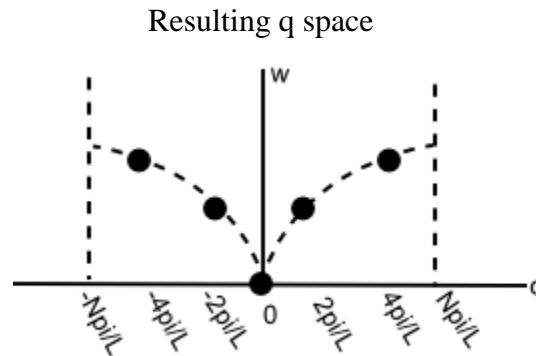
Summary: We begin these notes by finding a way to solve for allowed phonon modes in a finite crystal. We then give a couple of examples of this calculation. Next we introduce the density of states as a way to count the number of phonon modes per unit volume and solve for an expression for the density 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 $u_n = u_{n+N} = u_{n+2N} \dots$ 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 $1 = e^{iqNa}$
 - 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
 - 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 $q = \frac{2\pi}{Na} n_i = \frac{2\pi}{L} n_i$

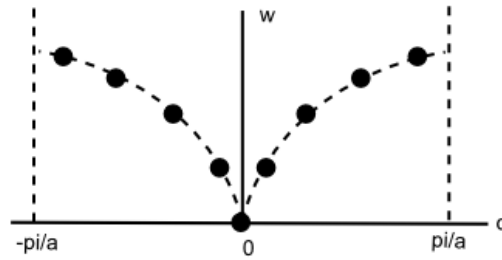


Example 2: Expanding out to a 1 cm long sample

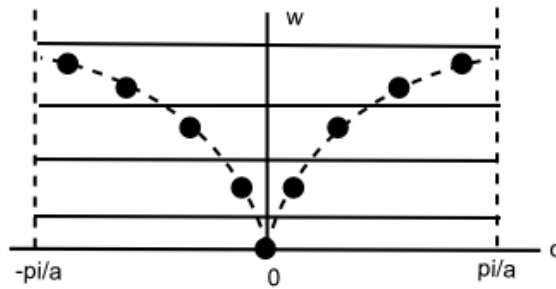
- Spacing between modes shrinks a lot, since L is much larger
- Brillouin zone stays the same (a unchanged) so there are a lot more modes in this sample
- Let $a=10^{-9}$ m and $L=10^{-2}$ m
- $N = \frac{L}{a}$ so 10^7 modes in this sample
- Although we drew the dispersion as a line it is actually made up of a *discrete* set of points
 - So close together they basically form a line

Density of states

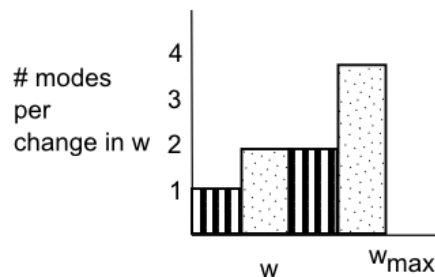
- Phonon dispersion can provide insight into material properties; however, the phonon dispersion is a non-trivial function in 3D and it is often helpful to bin modes by energy to simplify the description of what modes are present in a solid.
- The density of states is the number of modes within a E to $E+dE$ 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 ω , we want energy but this is just $\hbar\omega$ for our harmonic oscillator so to simplify just leave in terms of ω for one less variable....

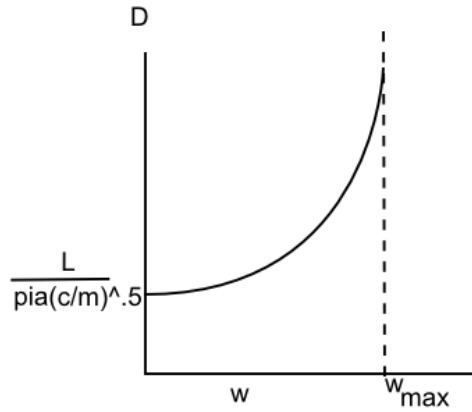


- Above is the binning of energy levels
- Now plot number of states versus omega



- 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 ω by taking the product of the density of states at a particular frequency ω 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 $d\omega/d\omega$
 - $D(\omega) d\omega = \frac{L}{\pi} dq \left(\frac{d\omega}{dq} \right) = \frac{L}{\pi} \left(\frac{d\omega}{d\omega/dq} \right) = \frac{L}{\pi} \left(\frac{d\omega}{v_g} \right)$ Group velocity v_g !
- Recall $v_g = \sqrt{\frac{c}{m}} a \cos\left(\frac{qa}{2}\right)$ 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 ω , 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* $D(\omega) d\omega = \frac{L}{\pi} \frac{d\omega}{a \sqrt{\frac{c}{m} - \frac{\omega^2}{4}}}$
- Plot D versus ω



- 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.

