

Topic 5-1: Introduction to Phonons
Kittel pages: 91, 92

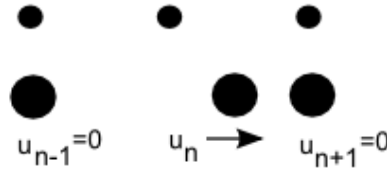
Summary: In this video we introduce the concept that atoms are not rigid, fixed points within the lattice. Instead we treat them as quantum harmonic oscillators, define a displacement as well as a force function, and use this to develop an expression for the dispersion relation for vibrations in a 1D chain of atoms. Finally, we give the dispersion physical meaning by giving examples of different displacement waves in this 1D chain.

- We will introduce vibrations in a lattice by treating atoms as simple harmonic oscillators instead of rigid, fixed points
- Quantum harmonic oscillators have a zero point energy at the ground state, which means there is motion even at 0 K
- This means crystals are inherently dynamic
- Start with a 1D crystal within a classical regime
 - Will treat bonds as springs
 - Only consider longitudinal vibrations which are vibrations that propagate along the direction of the crystal



- Put one atom at each lattice point so their spacing is given by a
 - The above figure shows one atom placed at each lattice point
 - The lattice point locations are given by the multiples of n above each atom
- Define position of atoms with no vibrations as x_n
- Also define u_n which is the displacement of atom n from the original configuration
- Can use Hooke's law for harmonic springs to approximate the force of the bonds on the atoms
 - $F=c\Delta x$ where c is the spring constant
- Need to be careful in defining Δx of the atoms

- In the figure below the top dots represent the lattice points. The larger dots are the atoms of which the outer two are still at their lattice points and the middle atom has oscillated off of its lattice point giving a non-zero displacement for this atom



- For the 1D chain, we can describe the force on atom n as:

$$F_n = c(u_{n-1} - u_n) + c(u_{n+1} - u_n) \quad [1]$$

- which is just the displacement of n relative to its two neighbors
- When all atoms have $u = 0$, they're all at their original lattice positions and $F_n = 0$.
- Need an expression for u_n
- **Approach:** Expect vibrations to travel as waves through the crystal, we'll use a traveling wave solution

$$u_n = u_0 e^{i(qx_n - \omega t)} \quad [2]$$

- Use q for our wave vector instead of k
- Now need an expression for force in terms of this traveling wave solution

- $ma = F$ where $a = \frac{\partial^2 u_n}{\partial t^2}$

$$m \frac{\partial^2 u_n}{\partial t^2} = c(u_{n-1} - u_n) + c(u_{n+1} - u_n) \quad [3]$$

- Inserting the traveling wave approach for u_n and rearranging we get

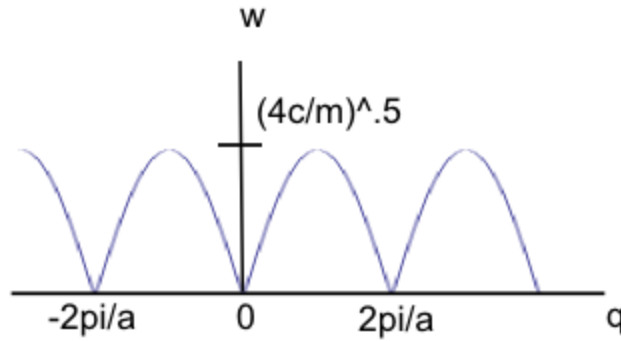
$$-m\omega^2 = c(e^{iqa} + e^{-iqa} - 2) \quad [4]$$

- Using Euler's formula we can get

$$-m\omega^2 = c(2\cos(qa) - 2) \quad [5]$$

- No longer have an explicit time dependence!!
- **Goal:** Develop a **dispersion relation** for vibrations in this 1D chain. A dispersion relation connects the wave vector (wavenumber q , in this 1D case) to the associated frequency of the mode.
- Rearranging $-m\omega^2 = c(2\cos(qa) - 2)$, we obtain:

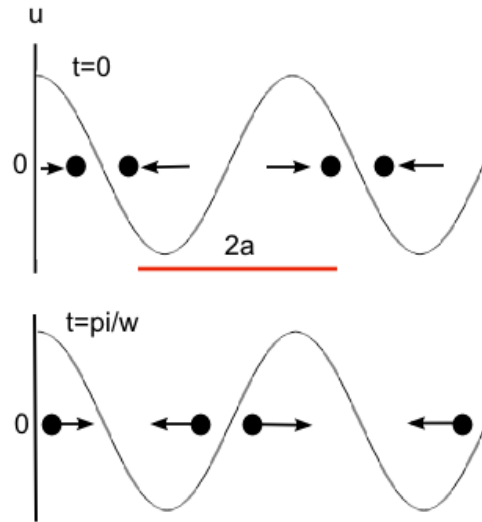
$$\omega(\vec{q}) = \sqrt{\frac{4c}{m} \left| \sin\left(\frac{qa}{2}\right) \right|} \quad [6]$$



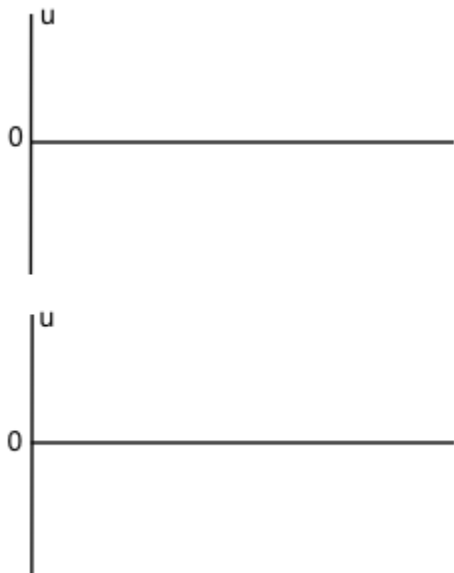
- With the dispersion relation we can relate q to ω ; however, this result doesn't immediately seem very interesting.
- **Goal:** Make the dispersion relationship have some physical significance
 - Putting the above expression which contains q into u_n ($u_n = u_o e^{i(qx_n - \omega t)}$), we get u_n in terms of ω and t instead of q and t
 - This has more physical significance! Let's see some examples:
- Example 1: Displacement wave with a long wavelength compared to lattice parameter a
 - Send in a sound wave
 - Wavelength can be anywhere from 20 mm to 20 m




- Atoms locally displacing nearly equal amounts at some time t
- $|\vec{q}| = \frac{2\pi}{\lambda}$, in this case q is really small
- So small that it barely shifts the dispersion off of the origin.
- Conclusion: The origin of the dispersion curve physically corresponds to extremely long wavelength waves; typically called acoustic waves
- Example 2: wavelength of displacement wave is $2a$ (shown in red, below)
 - This puts $|\vec{q}| = \frac{\pi}{a}$ which is at the local maximum of the dispersion relation
 - Atoms are completely out of phase with their neighbors



- Example 3: wavelength of $4a$
 - $|\vec{q}| = \frac{\pi}{2a}$
 - Partially out of phase motion
 - Just like above case but the nearest neighbors are less ‘in conflict’



 Sketch out a few time snapshots of these different wavevectors

- **General concept:** Why does the energy increase with increasing q ? As we move up the dispersion, we see that the atoms are more prone to be moving opposite their nearest

neighbors. Thus, they are compressing/expanding their springs significantly, increasing the energy of the mode.