Topic 5-3: Phonon Quantization
Kittel Pages: 99,100

Summary: In this video we begin by introducing quantization of lattice vibrations through quasi-particles called phonons. We then show that phonons carry no linear momentum. However, when they interact with other particles they act as though they do, hence the quasi-particle term.

- Difficult concept because we are talking about vibrational *waves* but describing them as a quasi-*particles*
  - Wave-particle duality!
  - Can compare with photons (both are bosons) - this means multiple phonons can occupy one mode
- Invoke that vibrations in a lattice behaves like harmonic oscillators
  - Energy of a particular mode

$$U(q) = (n(q) + \tfrac{1}{2})\hbar\omega(q) \qquad [1]$$

    - $\omega(q)$ is the frequency of oscillations of phonons with wavevector q, $n(q)$ is the population of phonons with wavevector q.
- **Physical picture:** Total amplitude of vibrational mode q in the lattice is related to $n(q)$. Later, we'll show that $n(q)$ scales with temperature. Hot solids have greater vibrational amplitude.
- Can prove this by looking at the kinetic energy density of the system

$$KE = \tfrac{1}{2}\rho(\tfrac{\partial u}{\partial t})^2 \qquad [2]$$

    - where ρ is the mass density

$$u = u_o \cos(qx)\cos(\omega t) \qquad [3]$$

    - u_o is the amplitude of vibration (non-complex version of the vibrational wave)
  - From the above two equations,

$$KE = \tfrac{1}{2}\rho(-u_o \cos(qx)\sin(\omega t))^2 \qquad [4]$$

$$\int_V d\vec{r}\, KE = \tfrac{1}{4}\rho V\omega^2 {u_o}^2 sin^2(\omega t) \qquad [5]$$

- Time averaged:

$$\text{KE} = \frac{1}{8}\rho V\omega^2 {u_o}^2 \quad [6]$$

- For a harmonic oscillator the total time averaged energy is divided evenly between kinetic and potential energy; aka it is half the total energy U.

$$KE = \frac{1}{2}U = \frac{1}{2}(n + \frac{1}{2})\hbar\omega \quad [7]$$

$$\frac{1}{8}\rho V\omega^2 {u_o}^2 = \frac{1}{2}(n + \frac{1}{2})\hbar\omega \quad [8]$$

$${u_o}^2 = \frac{4(n+\frac{1}{2})\hbar}{\rho V\omega} \quad [9]$$

- **Conclusions:** The amplitude of vibration (u_o) is proportional to the square root of the phonon population *n* for each mode q. Even if *n* = 0, u_o is non-zero!

Phonons and Linear Momentum

- Phonons carry no linear momentum
  - This is why they are called quasi-particles
  - Interact with other particles as though they have momentum when they really don't
- Analogous to hydrogen atoms oscillating in a hydrogen molecule
  - Hydrogen molecule has kinetic energy because of oscillations but the center of mass of the molecule never moves
- Just as for the hydrogen molecule, although a crystal's atoms are oscillating, over a time average there is no displacement of the crystal center of mass
- Need to prove lack of linear momentum

$$\rho = mv = m\frac{\partial}{\partial t}\sum_s u_n \quad [10]$$

  - sum is to add up all displacements before taking the time derivative

$$\rho = m\frac{\partial u_o e^{-i\omega t}}{\partial t}\sum_s e^{isqa} \quad [11]$$

  - Simplify using the infinite series approximation $\sum_{s=0}^{N-1} x^s = \frac{1-x^N}{1-x}$

$$\rho = m\frac{\partial u_o e^{-i\omega t}}{\partial t}\frac{1-e^{iNqa}}{1-e^{iqa}} \quad [12]$$

  - Boundary conditions on q to be discrete and $q = \pm\frac{2\pi n}{Na}$

- N is the number of atoms in the chain and n is an integer

$$\rho \propto \frac{1-e^{iNqa}}{1-e^{iqa}} \quad [13]$$

- where $q = \pm\frac{2\pi n}{Na}$
- $e^{iNqa} = e^{i2\pi n} = 1$

$$\rho \propto \frac{1-1}{1-e^{iqa}} = 0 \quad [14]$$

- Phonons carry no linear momentum!

Questions to Ponder

1. U is split evenly between kinetic and potential energy. Where are these energies represented in the system?

2. Why do phonons act like they have momentum when they interact with other particles?