Wed. Sept. 05

- Last time we began our disussion of how coupled QHO's affect the heat capacity of solids

- last time we considered a continuous solid medium of length L

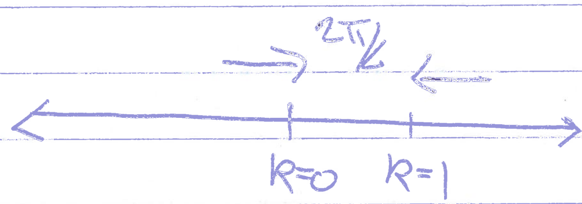
- using periodic boundary conditions only wavenumbers

$$k = \frac{2\pi n}{L} \qquad \left(\lambda = 2\pi/k \right)$$

wavelength

are "allowed"

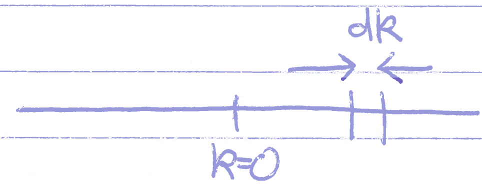
- each mode is a point in (1D) k-space



- what happens to the spacing between modes when $L \to \infty$?

- spacing becomes small + the points on k-axis become quasi-continuous

- We want to know the # of modes per "distance" along k-axis (density)
- How many modes exist in a segment dk?



- For large L, spacing between modes is small

$$\frac{L}{2\pi}\,dk = \#\text{ of modes in } dk$$

- Knowing the speed of sound for a solid, which is a material property, we may switch to frequency, ω of the modes by the dispersion relation

$$\omega = vk$$

- the "density of states" is the # of modes between ω + $\omega + d\omega$

$$g(\omega)\,d\omega = \#\text{ of states between } \omega + \omega + d\omega$$

- if $g(\omega)\,d\omega = \#$ of states

  $g(\omega)$ has units of $\frac{1}{(1/s)}$

- thus the term "density" (modes per freq.)

- now the # of modes in dk + # of states are related by

$$g(\omega)\,d\omega = \frac{L}{2\pi}\,dk$$

$$\Rightarrow g(\omega) = \frac{L}{2\pi}\frac{1}{d\omega/dk}$$

- if $\omega = vk \Rightarrow \frac{d\omega}{dk} = v$ (speed of sound)

$$g(\omega) = \frac{L}{2\pi}\frac{1}{v}$$

- each mode can move in + or − directions (mode → R or S)

- for each ω, two modes are possible

→

- Therefore, we actually have to multiply the right side by 2 (2 modes per ω)

$$g(\omega)\,d\omega = \frac{L}{\pi}\,dk$$

$$\Rightarrow \quad g(\omega) = \frac{L}{\pi}\frac{1}{v}$$

which is independent of ω

- on the homework, you will derive the density of states for the 3D case

volume of solid

$$g(\omega) = 3\frac{V}{2\pi^2}\frac{\omega^2}{v^2}$$

speed of sound

- notice $g(\omega) \propto \omega^2$ in 3D
- start by finding the # of modes in a sphere of volume defined by radius k in 3D k-space

- We will make use of density of states to further understand the specific heat in solids
- In Einstein's model, all oscillators have a common ω, which corresponds to T_E (Einstein temp.)
- Debye's model expands upon the success of Einstein's theory by assuming the oscillators are coupled
- From the dispersion relation $\omega = vk$ we have many ω's since for large L, we have many modes, k (v = const.)
- the lowest mode $k = 0 \Rightarrow \lambda = \infty$ is allowed, so state with $\omega = 0$ is possible (lowest state)
- how we determine the highest ω is more subtle
- our intution tells us $\omega \to \infty$ should not be possible (why?)
- So what is $\omega(\max)$?

- recall the expected value for the QHO

$$\langle E \rangle = \frac{1}{Z}\sum_n E_n e^{-\beta E_n}$$

$$= \frac{\hbar\omega}{e^{\beta\hbar\omega}-1}, \text{ or } \langle E \rangle = \langle E(\omega) \rangle$$

a function of ω

- quick check: high T regime
- let $x = \beta\hbar\omega$; $\frac{1}{e^x-1} \simeq \frac{1}{1+x-1} = \frac{1}{x} = \frac{1}{\beta\hbar\omega}$

$$\Rightarrow \langle E \rangle = \frac{\hbar\omega}{\beta\hbar\omega} = \frac{1}{\beta} = k_B T$$

(classical HO exp. value)

- What is the total energy of the solid? call it E
- We must add the energy of every state

$$E = \int_0^\infty \langle E \rangle g(\omega)\, d\omega$$

$g(\omega)$ → # of states with ω

$\langle E \rangle$ → Single oscillator with freq. ω

→

- so the total energy

$$E = \frac{3V}{2\pi^2 v_s^3} = \int_0^{\infty} \frac{\omega^2 \hbar\omega}{e^{\beta\hbar\omega}-1}\, d\omega$$

sound speed

- if we let ω $[0 \to \infty]$, we most certainly find $E \to \infty$
- but we already know $\omega \to \infty$ from physical arguments
- How do we determine ω_{max}?
- Debye argued

$$\int_0^{\omega_d} g(\omega)\, d\omega = 3N$$

where $N \equiv$ # atoms in a solid, thus giving $3N$ degrees of freedom

- ω_d is the "cutoff" frequency "Debye" freq.

• put $g(\omega) = \frac{3V}{2\pi^2} \frac{\omega^2}{V_s^3}$ into

$\int_0^{\omega_d} g(\omega) d\omega = 3N$ + solve for ω_d

$\omega_d = V_s (6\pi^2 n)^{1/3}$, where $n = N/V$ (density)

• now we may determine E knowing ω_d

from $E = \frac{3V}{2\pi^2 V_s^3} \int_0^{\omega_D} \frac{\hbar\omega^3}{e^{\beta\hbar\omega} - 1} d\omega$

+ $C_V = \frac{\partial E}{\partial T} = 3^2 R \left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx$

$x = \beta\hbar\omega$

or $C = N k_B \left[\frac{k_B T}{\hbar\omega_d}\right]^3 \frac{12\pi^4}{5} \sim T^3$

which captures the behavior at low T

- Debye's theory works very well to match experimental data (see handout)
- Some limitations are present, however:
- theory works up to T_0, but is not exact at intermediate temps.
- as we will discover $\omega = vk$ does not hold as the wavelength $\lambda \to a$, where a is the lattice spacing
- We will also find metals follow a slightly different behavior

$$C = \gamma T + \alpha T^3$$

where linear term dominates at very low T

- the origin of the liner term is free electrons in metals