Fri. Oct. 05

- We have been investigating the dispersion of a 1D solid with discrete nature (atoms)
- Using periodic boundary conditions, we see that

$$x_{n+N} = x_n$$

where N is the # of atoms & x_n is the position of atom 'n'

- we see that $u_n = u_{n+N}$ (disp. from eq.) on

$$Ae^{i(kx_n - \omega t)} = Ae^{i(kx_{n+N} - \omega t)}$$

- recall $x_n = na$ & $x_{n+N} = (N+n)a$

$$\Rightarrow Ae^{i(kna - \omega t)} = Ae^{i(k[N+n]a - \omega t)}$$

$$\Rightarrow e^{ikNa} = 1$$

$$\Rightarrow \cos(kNa) + i\sin(kNa) = 1$$

$$kNa = 2\pi p \quad (p \in \mathbb{Z} \text{ integers})$$

- therefore $k = \frac{2\pi p}{Na}$ or $k = \frac{2\pi p}{L}$

- where $L = Na$ is the total length of the solid

- so again, k values are discrete with spacing between k's being

$$\frac{2\pi}{L}$$

- we only count modes in first Brillouin zone

$$-\pi/a \leq k < \pi/a$$ (note don't double count mode at max. ω)

$$N = \frac{\text{range of } k\text{'s}}{\text{spacing between } k\text{'s}} \quad (\#\text{ of modes})$$

$$= \frac{2\pi/a}{2\pi/Na} = N$$

- just as was predicted by Debye //

- the energy of a lattice vibration is quantized & a quantum of such energy is called a phonon.

- given a mode with frequency ω, the energy is given by

$$E = \left(\frac{1}{2} + n\right)\hbar\omega$$

for excited state 'n', or the mode is occupied by 'n' phonons (quanta), $E = \hbar\omega$

- in analogy to classical physics, higher energy corresponds to larger amplitude of vibration (louder)

- each step up the ladder is a phonon

- we may have any number of phonons in the same state (bosons), just like photons

- Bose occupation factor

$$n_B(\beta\hbar\omega) = \frac{1}{e^{\beta\hbar\omega} - 1}$$

- so the expected value for a given mode

$$E_k = \hbar\omega(k)\left[n_B(\beta\hbar\omega(k)) + \frac{1}{2}\right]$$

- and of course the total energy is the sum of energies E_k

$$E_{total} = \sum_k \hbar\omega(k)\left[n_B(\beta\hbar\omega(k)) + \frac{1}{2}\right]$$

- the sum over k is for the first Brillouin zone only

- we know for real solid N is large

$$\sum_k \rightarrow \frac{Na}{2\pi}\int_{-\pi/a}^{\pi/a} dk$$

- check: $\frac{Na}{2\pi}\int_{-\pi/a}^{\pi/a} dk = N$

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- thus the total energy,

$$E_{total} = \frac{L a}{2\pi} \int_{-\pi/a}^{\pi/a} dk\, \hbar\omega(k) \left[n_B(\beta \hbar\omega(k)) + \frac{1}{2} \right]$$

- From which we may obtain the heat capacity

* note
see
page 5.5

- extending the analogy from photons, phonons also have momentum

$$\vec{p} = \hbar \vec{k}$$

which is called the "crystal momentum"

- this formulation allows us to treat phonons as particles

- for example, we see that phonons scatter from each other or phonons/photons interact etc.

- recall that for the continuum model the density of states

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

- for the 1D lattice:

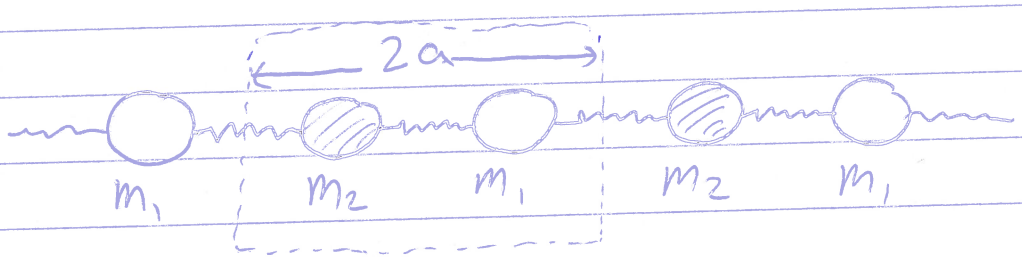
$$g(\omega) = \frac{2L}{\pi a \omega_{max}} \left[\cos\left(\frac{ka}{2}\right)\right]^{-1}$$

- Heat capacity

$$C_v = k_B \int \left(\frac{\hbar\omega}{k_B T}\right)^2 e^{\hbar\omega/k_B T} \left(e^{\hbar\omega/k_B T} - 1\right)^{-2} g(\omega) d\omega$$

- although it might seem pedantic to worry about what happens for a diatomic molecule, but some important physics is there

- Model: two repeating atoms of mass m_1 & m_2 in repeating units



- spring constant α is same

- the dashed box is our first encounter with a "unit cell" here of length '2a' (periodicity)

- Similar to our monatomic model we now have 2 diff. eqs.

over