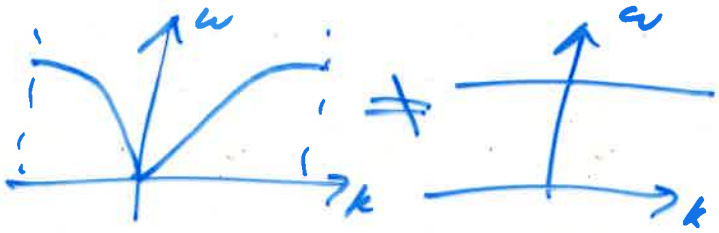
Einstein solid

N 3-dim SHO's $= 3N$ SHO's

one frequency $\omega = \omega_E$

Clearly not correct



$$E_a = \left(a + \tfrac{1}{2}\right)\hbar\omega$$

Partition function

$$Z = \sum_{a=0}^{\infty} e^{-\frac{E_a}{k_B T}} = \sum_{a=0}^{\infty} e^{-\frac{a\hbar\omega}{k_B T}} = \frac{1}{1 - e^{-\frac{\hbar\omega}{k_B T}}}$$

define $x = e^{-\frac{\hbar\omega}{k_B T}} \Rightarrow$

$$Z = \sum_{a=0}^{\infty} x^a \text{ - Geometric series} = \frac{1}{1-x}$$

Average Occupation number

$$\langle n \rangle = \frac{1}{e^{+\frac{\hbar\omega}{k_B T}} - 1}$$

Average energy for one SHO

$$\langle u \rangle = \langle \left(n + \tfrac{1}{2}\right)\hbar\omega \rangle = \langle n \rangle \hbar\omega = \frac{\hbar\omega}{e^{+\frac{\hbar\omega}{k_B T}} - 1}$$

Total energy for Einstein solid

$$U = 3N\langle u\rangle = \frac{3N\hbar\omega}{e^{+\frac{\hbar\omega}{k_BT}} - 1}$$

Heat Capacity constant volume (chain rule)

$$C_V = \left(\frac{\partial U}{\partial T}\right)_{NV} = \frac{3N\hbar\omega\,(-1)\,e^{+\frac{\hbar\omega}{k_BT}}\left(\frac{\hbar\omega}{k_BT^2}\right)(-1)}{\left(e^{+\frac{\hbar\omega}{k_BT}} - 1\right)^2}$$

$$= 3Nk_B\left(\frac{\hbar\omega}{k_BT}\right)^2 \frac{e^{\hbar\omega/k_BT}}{\left(e^{\frac{\hbar\omega}{k_BT}} - 1\right)^2}$$

$\lim_{T\to 0} C_V = 3Nk_B$ — Dulong-Petit

classical - Equipartition

$\lim_{T\to 0} C_V$ is exponential

But experiment is $\sim T^3$

We have ignored phonons. We only looked at oscillations of individual atoms, not 1000's of atoms.

$$U = \sum_k \sum_{p=1}^{3} \langle n_{kp} \rangle \hbar \omega_{kp}$$

p ← polarization

k ↖ wavevector

For N atoms, there are $3N$ wavenumbers

Easier to replace $\sum_k$ by integral

$$U = \sum_p \int d\omega \; D_p(\omega) \frac{\hbar \omega}{e^{\frac{\hbar \omega}{k_B T}} - 1}$$

↑ density of states

$D_p(\omega)$ is the number of vibrational modes (states) of polarization p in the frequency range ω to $\omega + d\omega$

$$D(\omega) = \frac{dN}{d\omega} \leftarrow \text{\# of states}$$

$$\int D(\omega)\, d\omega = \int \frac{dN}{d\omega} d\omega = \int dN = N$$

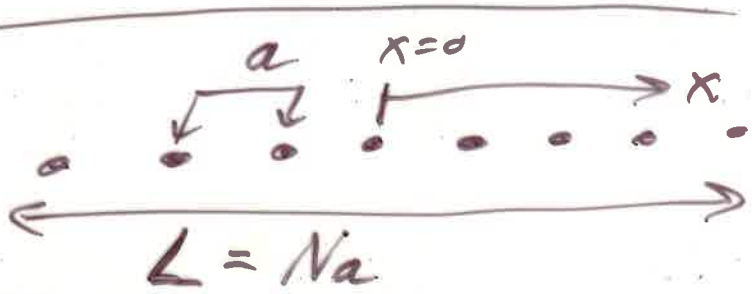
If $N(k)$ is the total number of states (modes) with wavenumber less than k.

$$D(\omega) = \frac{dN}{d\omega} = \frac{dN}{dk} \cdot \frac{dk}{d\omega} = \frac{dN}{dk}\left(\frac{1}{\frac{d\omega}{dk}}\right)$$

$$= \frac{dN}{dk} \frac{1}{v_{group}}$$

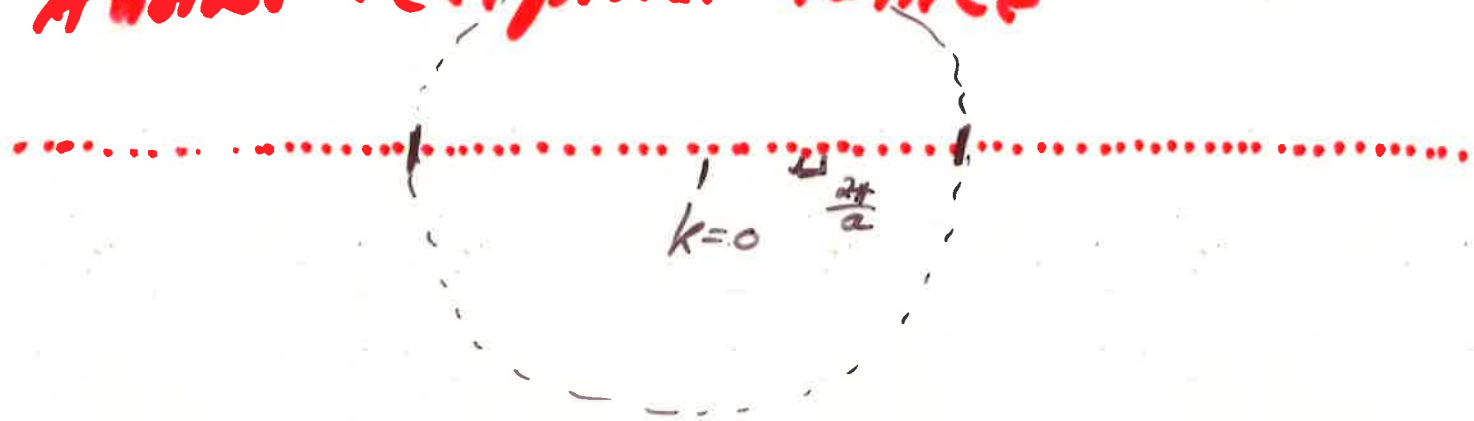
---

one dimension direct lattice



Reciprocal lattice

Another reciprocal lattice



$N(k)$ = # of dots (wavenumbers) in the interval.

$$N = \frac{L}{a} = \frac{Lk}{\pi} = \frac{2Lk}{2\pi} = 2k\left(\frac{L}{2\pi}\right)$$

$$\frac{dN}{dk} = 2\left(\frac{L}{2\pi}\right)$$

$$D(\omega) = \frac{dN}{dk}\cdot\frac{1}{v_g} = 2\left(\frac{L}{2\pi}\right)\frac{1}{v_{g\,map}}$$

Two dimensions

Direct lattice

Reciprocal lattice