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# Phys 425 Lecture 9

## Last time:

$$C_{solid} = 3R = 3Nk_B$$

## Einstein model

QSHO $\quad E_n = (n + \frac{1}{2})\hbar\omega$

↳ average over all states

$$\langle E \rangle = 3(\langle n \rangle + \frac{1}{2})\hbar\omega$$

↳ Bose - Einstein Distribution

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

$$C_{solid} = \frac{\partial \langle E \rangle}{\partial T}$$

$$\beta = \frac{1}{k_B T}$$

$$\boxed{C_{solid} = 3Nk_B(\beta\hbar\omega)\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}}$$

check: $k_B T \gg \hbar\omega \Rightarrow C_{solid} \to 3Nk_B$

So, Dulong-Petit model is correct at high Temp limit.

↳ didn't account for that low temperatures "freeze" alot of the classical degrees of freedom.

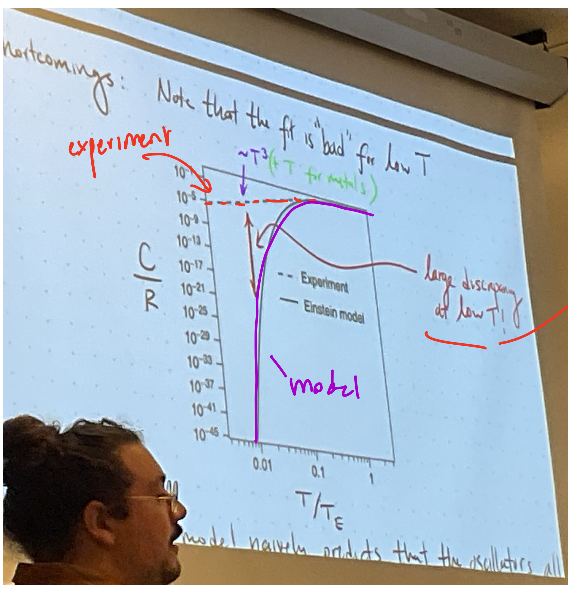
d.o.f. = temperature dependent

## Einstein Model:

- single fitting parameter, $\omega_E$ = Einstein freq.

$$\hbar \omega_E = k_B T_E$$

Einstein frequency, Einstein temperature.

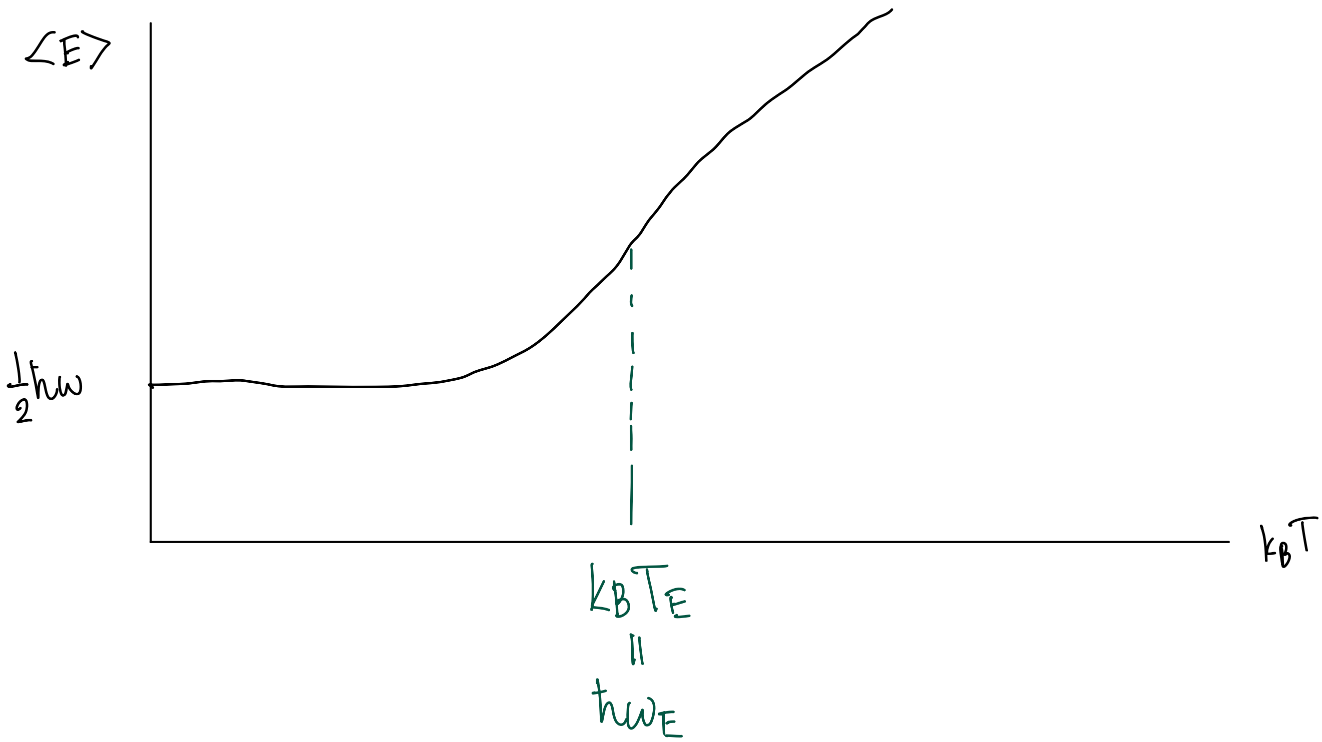



large discrepancy at low T

## Shortcomings of the Einstein model:

1. $T^3$ dependence predicted by experiments @ low T
   - ↳ Einstein's is exponential

2. Einstein model, naively, predicts anything below that temperature will exponentially fall to the ground state.




3. Einstein assumes no interaction between the atoms.
   - assume independent oscillators
   - ↳ incorporate lattice somehow to get a better approximation

4. Assuming that $\omega$, the frequency of the oscillators, is constant.
   - Not true at all
   - we in fact have a spectrum of $\omega$s

# Debye Model

## Debye's idea:

- treat oscillations as a sound wave
  $\hookrightarrow V_s = \frac{\omega}{k}$

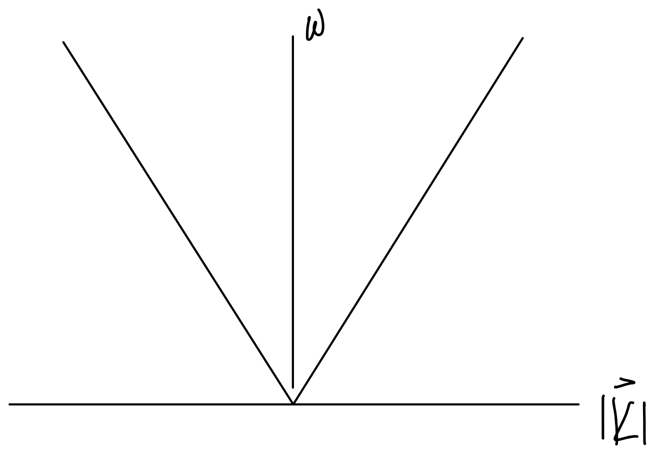
  Dispersion Relation $\omega(\vec{k}) = v|\vec{k}|$

## Einstein

- was 3N oscillators
  w/ freq (constant)

## Debye Model

3N oscillators
w/ freq
$\omega = v|\vec{k}|$




$$\langle E \rangle = \sum_{|\vec{k}|} \left( \langle n(\omega(\vec{k})) \rangle + \frac{1}{2} \right) \hbar \omega(\vec{k})$$

$$\langle n(\omega(\vec{k})) \rangle = \frac{1}{e^{\beta\hbar\omega(k)} - 1}$$

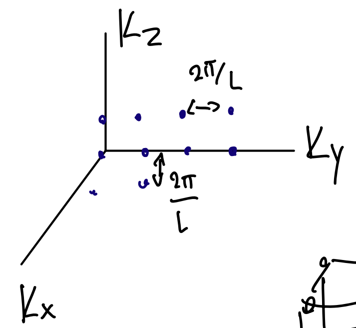
# ASIDE

## Periodic Boundaries:

If we assume the length of the solid is large enough,

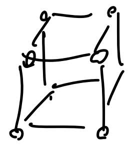
we can turn the $\sum_{\vec{k}} \Rightarrow \int dk$

In $\vec{k}$-space,




$\vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$

integer



$\text{Vol} = \left(\frac{2\pi}{2}\right)^3$

As $L \to \infty$, $\text{vol} = \left(\frac{2\pi}{L}\right)^3 \to 0$

So $\sum_{|\vec{k}|} \to \left(\frac{L}{2\pi}\right)^3 \int (\ \ ) dk$

generally, $\text{vol} = \left(\frac{2\pi}{L}\right)^d$

1 state allowed in this volume.

To get our energy $\langle E \rangle$

we need density of states:

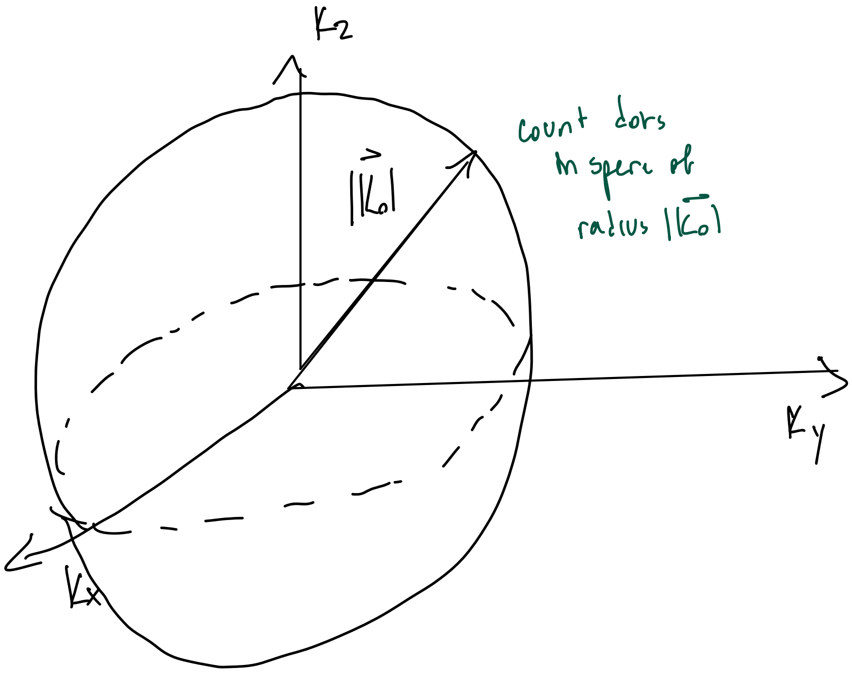
↳ sum all states in some volume up to some $\vec{k}_0$

$$N = \sum_{|\vec{k}| \leq |\vec{k}_0|}$$

We saw

$$g(\omega) = \frac{dN}{d\omega}$$

3D:




$$N = \sum_{|\vec{k}| \le |\vec{k}_0|} 1 \rightarrow \left(\frac{L}{2\pi}\right)^3 \int_{\text{sphere}} d^3k = \left(\frac{L}{2\pi}\right)^3 \int_0^{2\pi}\int_0^{2\pi}\int_0^{k_0} k^2 \sin\theta \, dk \, d\theta \, d\phi$$

$$= \left(\frac{L}{2\pi}\right)^3 4\pi \int_0^{|\vec{k}_0|} k^2 \, dk$$

Change variables:

$$\omega = v|\vec{k}|$$ main assumption of this model

$$N(\omega) = \left(\frac{L}{2\pi}\right)^3 4\pi \int \frac{\omega^2}{v^3}$$

$$\hookrightarrow \quad g(\omega) = 3\left(\frac{L}{2\pi}\right)^3 \frac{4\pi\omega^2}{v^3}$$

include degrees of freedom (polarizations)

$$\langle E \rangle = \int E' \, g(E') \, n(E) \, dE$$

$$\int 3\left(\frac{L}{2\pi}\right)^3 \cdot \frac{4\pi\omega^2}{v^3} \left( \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} + \frac{\hbar\omega}{2} \right) d\omega$$