Phys 425

Lecture 10

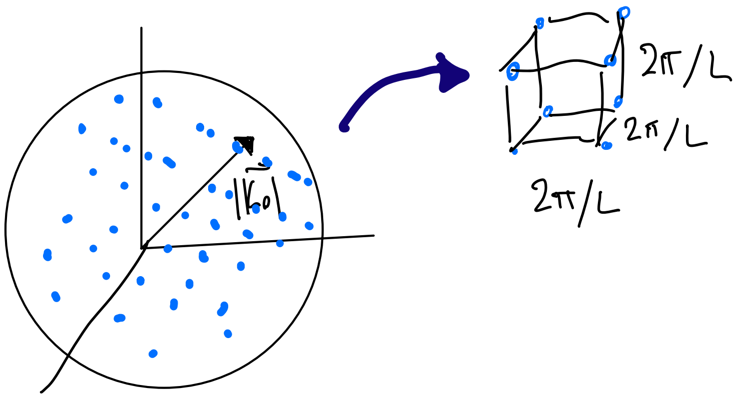
Debye model:

Dispersion Relation

$\omega(\vec{k}) = V|\vec{k}|$ "sound waves"

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

count # of states up to some cutoff $\overline{K_o}$



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

$$N = \sum_{\vec{k} \leq |\vec{K_o}|} 1$$

states within the sphere

L: size of your system

solid of $L \times L \times L$,

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

Einstein assumed ω was constant

↳ It wasn't

experimental data showed it should be a T^3 dependence.

Now we need a density of states

- cut off all the Ks within some volume (trace out a sphere)

K states are dots within the sphere

$$N = \sum_{\vec{k} \leq |\vec{k}_0|} 1 \quad \text{\# of states within sphere} \quad = \left(\frac{L}{2\pi}\right)^3 \int d^3k$$

$g(w) \to 3D$

$$N = \int \boxed{3\left(\frac{L}{2\pi}\right) \frac{4\pi w^2}{v^3}} \, dw$$

accounts for d.o.f (polarizations)

$$g(w) \equiv \text{density of states} = \frac{dN}{dw} \Rightarrow N = \int g(w)\,dw$$

$$g_{3D}(w) = \underbrace{3}_{\substack{\text{d.o.f} \\ \text{(polarization)}}} \underbrace{\left(\frac{L}{2\pi}\right)^3}_{\substack{\text{density of} \\ \vec{k} \text{ states in} \\ \vec{k} \text{ space}}} \underbrace{\frac{4\pi w^2}{v^3}}_{\substack{\text{volume of} \\ \text{a sphere of some} \\ \text{radius } \vec{k}_0}}$$

Now that we have the density of states:

Now we calculate $\langle E \rangle$

If we know $g(w)$, then

$$\langle E \rangle = \int \underset{\substack{\parallel \\ \hbar w}}{E}\, g(w)\, n(w)\, dw$$

we can also use the $\langle E \rangle$ from before

$$\langle E \rangle = \sum_{\vec{k}} \hbar w(\vec{k}) \left(\frac{1}{e^{\beta \hbar w(\vec{k})} - 1} + \frac{1}{2} \right)$$

Same method to get to $g(w)$

pushed $\hbar\omega$ into integral

E_{phonon}

$$\langle E \rangle = \underbrace{\boxed{3\left(\frac{L}{2\pi}\right)^3 \frac{4\pi}{v^3} \int_0^\infty \omega^2}}_{g(\omega)} \left(\boxed{\hbar\omega} \underbrace{\frac{1}{e^{\beta\hbar\omega} - 1}}_{\text{Bose Einstein distribution}} + \frac{\hbar\omega}{2} \right) d\omega$$

let x be $\beta\hbar\omega \rightarrow dx = \beta\hbar d\omega$

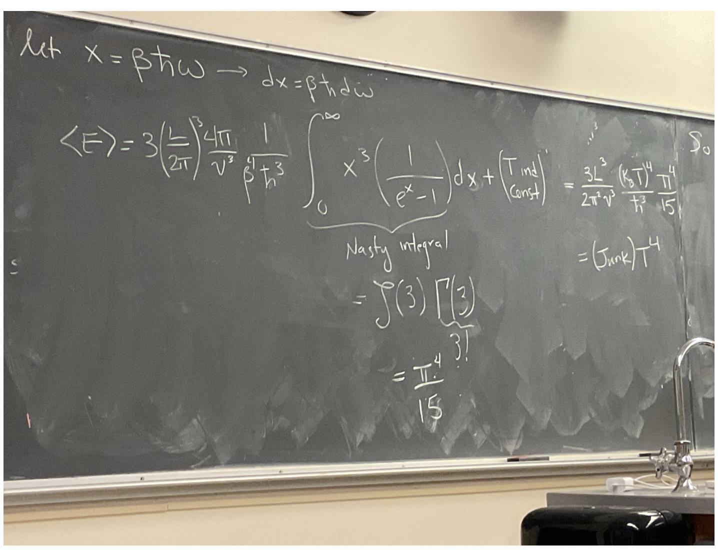
$$\langle E \rangle = 3\left(\frac{L}{2\pi}\right)^3 \frac{4\pi}{V^3} \left(\frac{1}{\beta^4 \hbar^3}\right) \int_0^\infty \underbrace{x^3 \left(\frac{1}{e^x - 1}\right)}_{\text{Nasty integral}} d\omega + T_{ind} \text{ constant}$$

$$\hookrightarrow \zeta(3)\underbrace{\Gamma(3)}_{3!}$$

$$= \frac{\pi^4}{15}$$

$$C = \frac{\partial E}{\partial T}$$

$$= \frac{3L^3}{2\pi^2 V^3} \frac{(k_B T)^4}{\hbar^3} \frac{\pi^4}{15} = (\text{Junk}) T^4$$



$\langle E \rangle \propto T^4$!

$\Downarrow$

$$C = \frac{\partial \langle E \rangle}{\partial T} \propto T^3$$

$$\frac{3L^3}{2\pi^2 V^3} \frac{k_B^4}{\hbar^3} \frac{\pi^4}{15} 4 \cdot T^3$$

So we have found the source of the T^3 behavior, the source of the ω is not constant.

(Is this good for all T)

The problem: We need to localize or restrict T^3 behavior to low T (temperature)

The fix: introduce another cutoff:

$W_D \rightarrow$ Debye Frequency

↳ caps # of states allowed to just the total # of d.o.f.

$3N \rightarrow$ 3 for the dimensions
N for the total states in the solid

$$3N = \int_0^{W_D} g(w)\,dw$$

# of states

$$\boxed{W_D = \frac{V}{L}\left(6\pi^2 N\right)^{1/3}}$$

Check: This cutoff also recovers the Dulong Petit Prediction @ high temperatures.

$C \rightarrow 3Nk_B$

@ T_{LARGE}

$$\langle E \rangle = \int_0^{\omega_D} g(\omega) \frac{\hbar\omega}{e^{\beta\hbar\omega}-1}\, d\omega + \text{const}$$

$$\Rightarrow \quad C = 9 N k_B \left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} \frac{x^4 e^x}{(e^x-1)^2}$$

$$\hbar\omega_D = k_B T_D$$

T_D : T debye