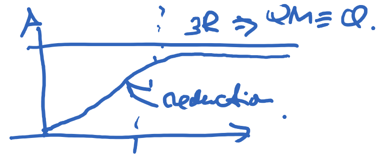
Thursday, April 09, 2020 1:59 PM

Lecture 19, April 9, 2020

$$E = E_0 + \sum_{f \leftarrow \text{modes}} \hbar\omega \langle n_f \rangle$$

$$\langle n_f \rangle = \frac{1}{e^{\beta\hbar\omega} - 1}$$

$$\left.\frac{\partial E}{\partial T}\right|_{V=\text{const}} = C_V$$



$3R \Rightarrow$ QM $\equiv$ CQ.

reduction

$$\boxed{C_V = \frac{\partial}{\partial T} \sum_f \hbar\omega_f \langle n_f \rangle}$$

1. high T limit $kT \gg \hbar\omega_f$

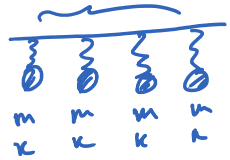
$\underbrace{C_V = kN3}$ $\leftarrow$ for a mole.

Dulong-Petit result.

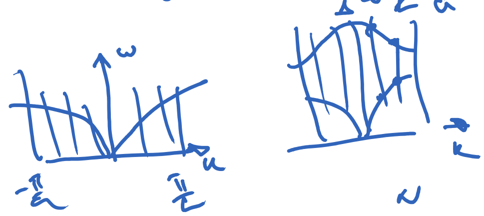
2. what to do when $T \to 0$?

Einstein model (naivé)

real oscillator.



$$\equiv \left(\ \right)^N \qquad \omega_0 = \sqrt{\frac{k}{m}}$$



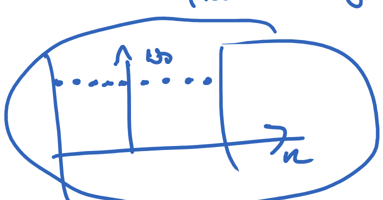
$\Delta\omega$ opt oscillators are fake.

$$E = 3N \frac{\hbar\omega_0}{e^{\hbar\omega\beta} - 1}$$

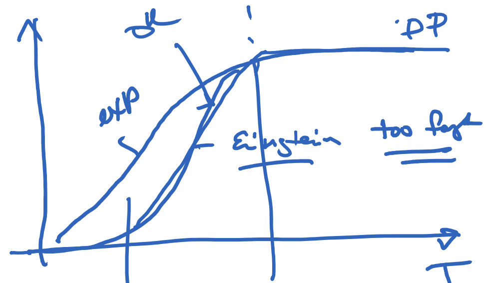
The sum of 3N identical terms

N points (N # of cells on the ring ~~of the PBC~~)

N all 1 .. 1



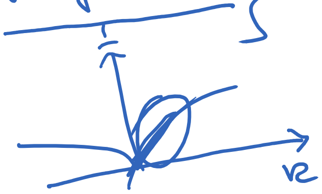
$$C_V = \frac{3N (\hbar\omega)^2 e^{\hbar\omega\beta} / (kT)^2}{\left[e^{\hbar\beta\omega} - 1\right]^2}$$

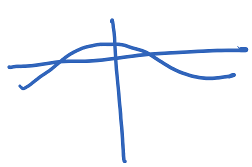


There is nothing to excite thermally!

2 Springs

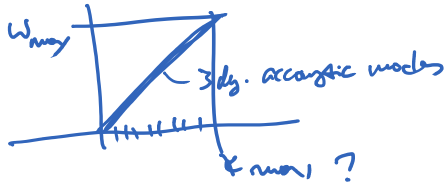
very stiff

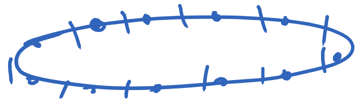




Debye

Debye





N cells (one atom per cell for simplicity)

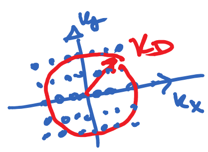
$\omega = c * k$

$N\left(\frac{2\pi}{L}\right)^3$ = volume of k-space to hold all solutions allowed by PBC.

assume BZ to be a sphere.
The radius of it is $K_{max} = k_D$ $\Rightarrow$ $\frac{4}{3}\pi k_D^3$ — this is the volume of the 1st BZ where all my solutions live.

$\boxed{L^3 = V}$

$$\frac{4}{3}\pi k_D^3 = \frac{N}{V} 8\pi^3$$



$\frac{N}{V} = n \Rightarrow \boxed{k_D^3 = n\, 6\pi^2}$

all allowed k-points

$$\underbrace{\sum_k 1 = N_{cells} = \frac{V}{(2\pi)^3}\int d^3k}$$

$\sum_F$ sum over all modes!

$$C_V = \frac{\partial}{\partial T} \sum_{br.} \int \frac{d^3k}{(2\pi)^3} \frac{\hbar\omega(k)}{e^{\hbar\omega(k)\beta} - 1} = \frac{\partial}{\partial T} 3 \int_0^{k_D} \frac{k^2 dk}{8\pi^3} 4\pi \frac{\hbar c k}{e^{\hbar c k \beta} - 1} =$$

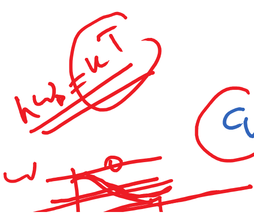
branches? only 3, and they are identical.

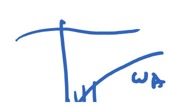
$$= \left\{ x = \frac{\hbar c k}{kT} \right\} = 9 n k \left(\frac{T}{\Theta}\right)^3 \int_0^{\Theta/T} \frac{x^4 e^x dx}{(e^x - 1)^2}$$

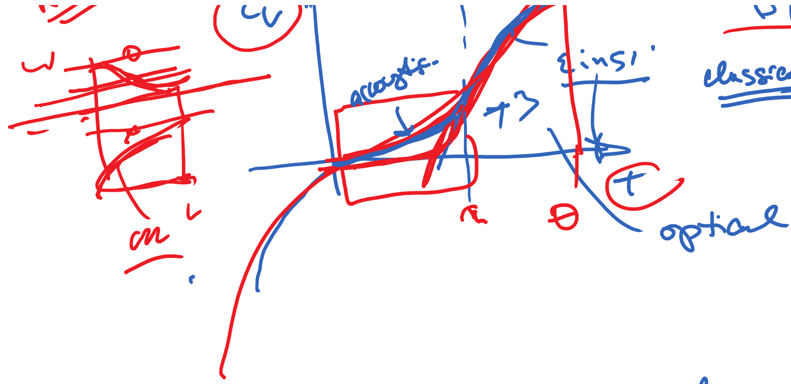
evaluate numerically.

$$\Theta_D = \frac{\hbar c k_D}{k_B}$$

$\boxed{C_V \sim T^3}$







classical $\equiv \Theta$

$\left|\sum_i \mathcal{P}_{AB}\right|^2 =$

$k \to 0$

$\omega \to 0$

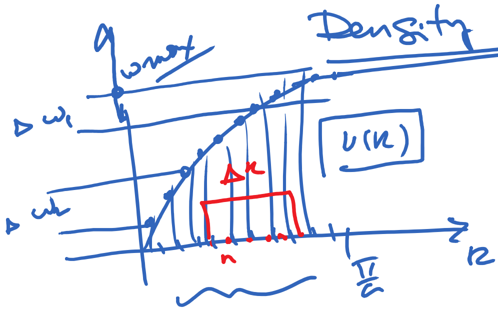
$\frac{2\pi}{L}$ $\left(\frac{2\pi}{L}\right)^3$

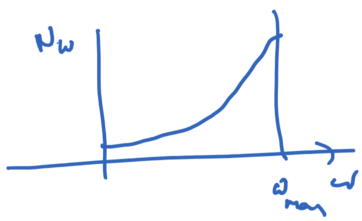
\# of k points.

$L \to \infty \equiv N_{cells} \to \infty$

Σ ← Thermodynamic limit

Density of States





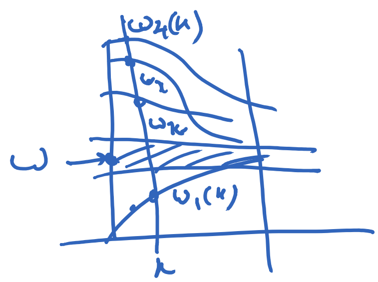
$\omega(k)$ determines the DOS in ω !

Separate by $\left(\frac{2\pi}{L}\right)$ Δk

$$\frac{\Delta n}{\Delta k} = \frac{L}{2\pi} \quad D(k)$$

$\Delta n \times \frac{2\pi}{L} = \Delta k$

A Formal connection



$$\sum_s \frac{V}{(2\pi)^3}\int d^3k\, F(\omega) = V\int d\omega\, D(\omega)\, F(\omega)$$

br. index. $\omega_s(k)$

$F(\omega_1(k)),\ F(\omega_2(k))\ldots$

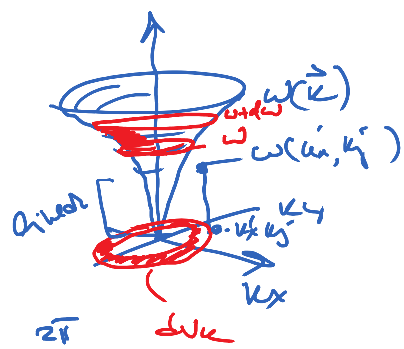
defines $D(\omega)$

$$\boxed{D(\omega) \equiv \sum_s \int \frac{d^3k}{(2\pi)^3}\,\delta(\omega - \omega_s(k))}$$

→ This is a counter! every time you hit the eigenvalue $\omega_s(k)$ you increment.

More intuitive form of $D(\omega)$.

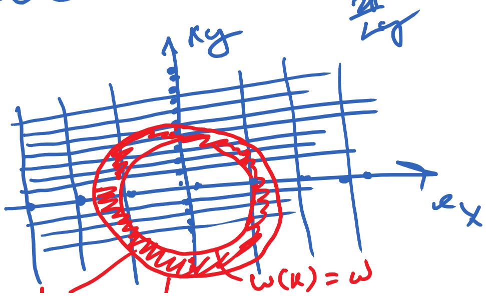
for simplicity, let's do 2D.



$\omega = \omega(k)$

$\omega + d\omega = \omega(k) + d\omega$

$$\boxed{D(\omega)\,d\omega = \frac{A}{(2\pi)^2}\, dA_k}$$



$$\boxed{D(\omega)\,d\omega = \frac{A}{(2\pi)^2}\, dA_k}$$

k_x 2_x

$$\left[D(\omega)\,d\omega = \frac{V}{(2\pi)^3}\, dV_k\right]$$

2D : $\frac{1}{A} D(\omega)\,d\omega = \frac{dA_k}{4\pi^2}$

3D : $\frac{1}{V} D(\omega)\,d\omega = \frac{dV_k}{8\pi^3}$

$dA_k = d\vec{k}\cdot d\vec{l}$

in 3d $dV_k = d\vec{k}\cdot d\vec{S}$

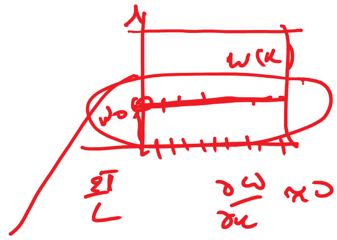
$\omega(k)$ we know that!

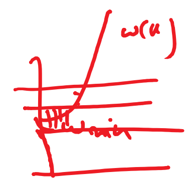
$k \to k+\Delta k$ how much ω changes? $\Delta\omega = \frac{\partial\omega}{\partial k}\Delta k$

$\lim \Delta k \to 0 \;\to\; d\omega = \nabla_k\omega \cdot d\vec{k}$ $\qquad dV_k = d\omega \int \frac{dS}{\nabla_k \omega}$

3D: $$\boxed{D(\omega) = \frac{1}{8\pi^3}\int \frac{d\vec{S}}{|\nabla_k \omega(k)|}}$$

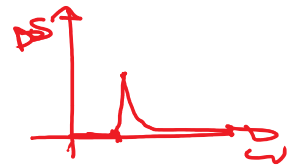
2D : $$D(\omega) = \frac{1}{4\pi^2}\int \frac{d\vec{l}}{|\nabla_k \omega(k)|}$$





$\frac{2\pi}{L}$ $\qquad \frac{\partial\omega}{\partial k} \approx 0$ $\qquad \frac{\partial\omega}{\partial k} = \text{LARGE \#}$

$D(\omega) \sim \infty$ $\qquad D(\omega)$ small

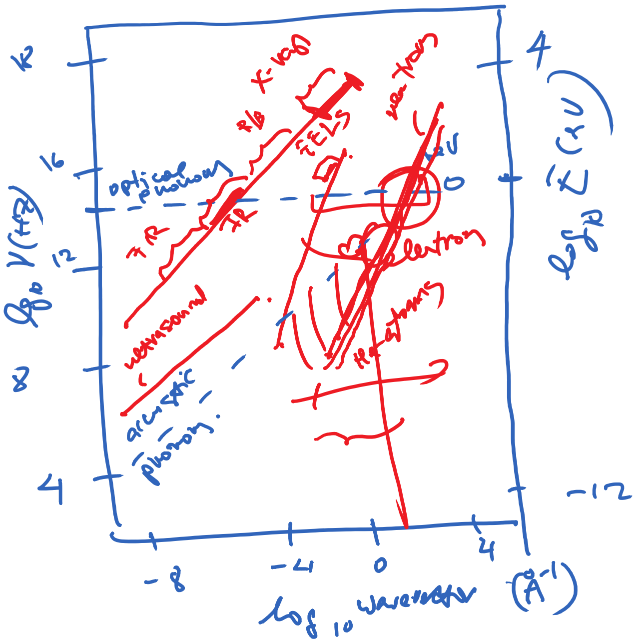


Experimental Techniques to study phonons:

scattering - based techniques.

$E_p = E_{ex} \leftarrow$ { elastic / non-elastic. -x-ray }

$k_p = k_{ex.} \leftarrow$ always true.



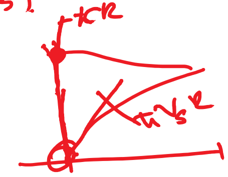
1. IR Spectroscopy.

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

2. Raman Scattering

(Stokes, anti-Stokes)

Optical phonons.



- Brillouin Spectroscopy.

  acoustic mode.

- x-ray — not great

- Inelastic neutron Scattering.

  ↳ work-horse of phonon measurements.

  Energy and momentum are well matched for $\hbar\omega_q$.