In class 4/19/23

$V_0 + \sum_{j=1}^{3N} \frac{\partial V}{\partial x_j}\Big|_{x_{c0}} x_j + \frac{1}{2}\sum\sum \frac{\partial^2 V}{\partial x_j \partial x_i}$

1) $\ln Q = -\beta E_0 + \int_0^\infty \ln(1-e^{-\beta\hbar\omega})\, g(\omega)\, d\omega$ ← when quant

$V = V(\underbrace{x_1, x_2, x_3}_{\text{atom pos}} \ldots x_{3N})$

2) $g(\omega)\,d\omega$ = binning close Q states in order to restate $\sum_{j=1}^{3N} \ln(1-e^{-\beta\hbar\omega_j})$ form, $\boxed{g(\omega)\,d\omega}$ = no. of phonons in V w/ ω in $[\omega, \omega+d\omega]$

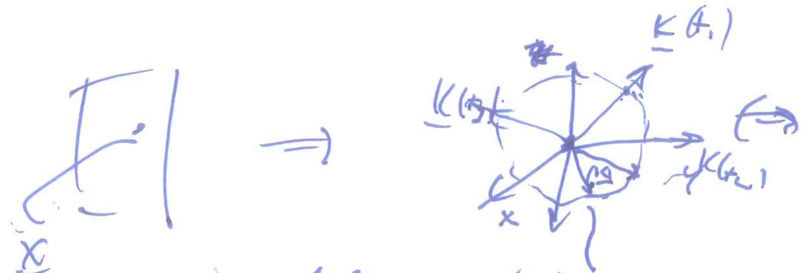
$\underbrace{V_0 + \sum_{j}^{3N} \frac{1}{2}\hbar\omega_j}_{\text{Binding energy}}$

3) Time: MATH

$$\boxed{n_{\underline{dk}} = \frac{V}{2\pi^3}\, \underbrace{dk_x\, dk_y\, dk_z}_{d\underline{k}}}$$

= no of phonon modes in V, ~~per~~ ~~phonon~~ w/ $\underline{k}$ in $[\underline{k}, \underline{k}+\underline{dk}]$

4) At only $\underline{x}$ in V, assume phonon wave vecs. are isotropic



@ $\underline{x}$, measure (somehow) wave ~~fronts~~ vectors over time and get this

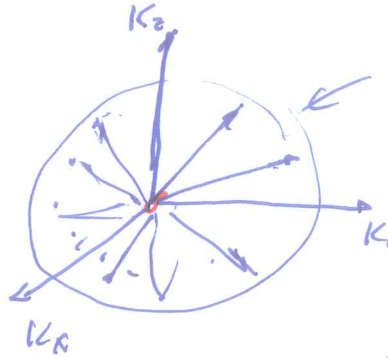
time avg distbn of $\underline{k}$'s

For any $|\underline{k}| = k$, the ~~time~~ ~~avg~~ distbn of $\underline{k}$'s observed over long times is uniform over a sphere of radius $|\underline{k}| = k$

5) Now find total no. of phonons in V having $|\underline{k}|$ in $[|\underline{k}|, |k| + |\underline{dk}|]$:

$\boxed{g(\omega)\, d\omega}$

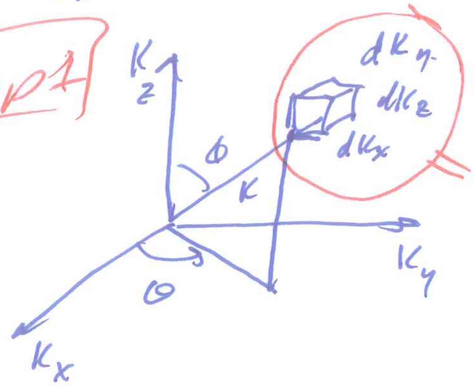
a) At any $\underline{x}$ we have following picture: in "$\underline{k}$-space":



random distbn of observed $\underline{k}$'s @ $\underline{x}$

$\Rightarrow$ $[\Delta \underline{k}] = [dk_x, dk_y, dk_z]$

step 1



@ $N_{\Delta k} = \frac{V}{(2\pi)^3} \underbrace{dk_x dk_y dk_z}_{[\Delta k]}$

= no phonon modes, in V, @ any $\underline{x}$, w/ $\underline{k}$ in $[\underline{k}, \underline{k} + \underline{dk}]$

b) $|\Delta \underline{k}| = k^2 \sin\phi \, d\theta \, d\phi \, dk$

c) Let N_k = tot no. of phonon modes in V, @ any $\underline{x}$, w/ $|\underline{k}| \equiv k$ in $[k, k + |\underline{dk}|]$.

$$N_k = \frac{V}{(2\pi)^3} \int_0^{\pi} \int_0^{2\pi} d\theta \, k^2 \, dk \, \sin\phi \, d\phi$$

d) $\boxed{N_k = \frac{V}{(2\pi)^3} 4\pi k^2 \, dk}$

e) $\therefore \boxed{g(K)\,dK \equiv N_K = \frac{V}{(2\pi)^3} 4\pi K^2 dK}$ 3

f) Assume that each phonon corresponds to a continuum elastic sound wave

$\lambda_{min} \sim 10 a_0 \sim 10 (4\,\text{Å})$

$\sim 4\,nm$

$\therefore$ For $\lambda \gg \lambda_{min}$,

$$c_l = \frac{\omega}{K}$$

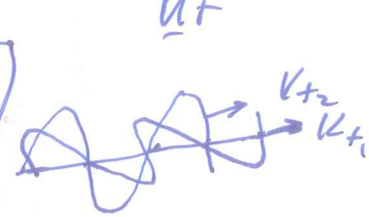
Ref : pg 412-413 — (8) (399)

a)

$$\boxed{\frac{1}{c_\ell^2}\underline{u}_{\ell,tt} = \nabla^2 \underline{u}_\ell \qquad \frac{1}{c_t^2}\underline{u}_{t,tt} = \nabla^2 \underline{u}_t}$$

b) $|\underline{k}_\ell| = \boxed{\frac{\omega}{c_\ell} = k_\ell}$

$|\underline{k}_t| = \boxed{\frac{\omega}{c_t} = k_t} \Rightarrow$



c) $\underline{u}_t \cdot \underline{k}_t = 0 \Rightarrow$ u_t reps displacement $\perp$ to $\underline{k}_t$

$\underline{u}_\ell \parallel \underline{k}_\ell$

d) $g_\ell(\omega)\,d\omega = \frac{V}{(2\pi)^3} 4\pi k_\ell^2 \, dk_\ell$ = total no. of long. elastic sound waves in V in $[k_\ell, k_\ell + dk_\ell]$

$g_t(\omega)\,d\omega = (2)\frac{V}{(2\pi)^3} 4\pi k_t^2 \, dk_t$ = total no. transverse elastic sound waves in V in $[k_t, k_t + dk_t]$

d')

$$\boxed{g_\ell(\omega)\,d\omega = \frac{V}{(2\pi)^3}(4\pi)\left(\frac{\omega^2}{c_\ell^3}\right)d\omega}$$

$$g_t(\omega)\,d\omega = \frac{V(2)4\pi}{(2\pi)^3}\frac{\omega^2}{(c_t^3)}\,d\omega$$

⑤

∴ g) $g_{\substack{\text{Band}\\ \text{effective}}}(\omega)\,d\omega = [g_\ell(\omega) + g_t(\omega)]\,d\omega$

$$\equiv \boxed{\frac{3V}{(2\pi^2 c^3_{\text{eff}})}\,\omega^2\,d\omega}$$

$$\boxed{\frac{3}{c_{\text{eff}}} = \frac{1}{c_\ell^3} + \frac{2}{c_t^3}}$$

$$\text{II)}\quad \boxed{-\int_0^{\omega_D} \ln\left(1 - e^{-\beta\hbar\omega}\right)\frac{3V\omega^2}{2\pi^2 c^3}\,d\omega}$$

$\therefore \ln Q = -\beta G_0$

B) $\boxed{\omega_D}$ = Debye freq

$$\int_0^{\omega_D} g(\omega)\,d\omega = 3N$$

or $$\int_0^{\omega_D} \frac{3V}{2\pi^2 c^3}\,\omega^2\,d\omega = 3N$$

or $$\omega_D^3 = \frac{3Nc^3(2\pi^2)}{V}$$

or $$\omega_D = (6\pi^2)^{1/3}\left(\frac{N}{V}\right)^{1/3} c$$

$$\sim (3.7)\left(\frac{1}{a_0}\right)c \sim \frac{3.7\ \ 5(10^3)\ \text{m/s}}{4(10^{-10})\ \text{m}} \sim 5\,(10^{13})\ \text{s}^{-1}$$

prev works

Q2 $\quad \omega_D = \omega_{max} = (6\pi^2)^{1/3} \left(\frac{N}{V}\right)^{2/3} c$

$\sim \frac{c_{sound}}{a_0} \sim \frac{5(10^3) m}{4(10^{-10})}$

~~For~~ ~~$\omega \gg \omega_D$~~

For T

$\boxed{\omega_{max} \sim 10^{13} s^{-1}}$

(1)

$\Rightarrow k_B T_D = \hbar \omega_D$

$\omega_D = fn(\text{props})$

$T_D = \hbar \omega_D / k_B = fn(\text{material})$ coll...

$T_{D_{metals}} \sim 400\text{-}600 K$

$T_{D_C} \sim 2000K \Rightarrow$

For $T > T_D$ what happens i.e. where does thermal energy get dumped

what happens for $T > T_D$ ($\Leftrightarrow$ phonon energies) Bose $\hbar \omega_{max}$

A1 phonon model:

$E_{sys_j} = V_0 + \frac{1}{2}\sum_j^{3N} \hbar \omega_j +$

$n_1 \hbar \omega_1 + n_2 \hbar \omega_2 \ldots$

B1

$n_1 = 0, 1, 2 \ldots$ 3N

sound   Al

$\hbar\omega$

1   $\omega_{max} \sim c/a_0 \sim \frac{5(10^3)\,m/s}{3(10^{-10})}$

space $\sim \boxed{2(10^{13})\,s^{-1}}$

Q1 what ω's do n'3 look like as fn of ω max T

II

$\frac{2\pi \text{ rads}}{\text{cycle}} \frac{\text{cycle}}{s}$ $\nu =$ cycle/s

$\omega_{min} \sim c/L \sim \frac{5(10^3)\,m/s}{3\,10^{-2}\,m}$ 2

$\sim 2(10^5)\,s^{-1}$

$\epsilon_{min} \sim \hbar\omega_{min} \sim 10^{-34}\,Js\,(2)(10^5)\,s$

$\sim 10^{-29}\,J$

$\epsilon_{max} \sim \hbar\omega_{max} \sim$

$K_B T \sim \hbar\bar{\omega}_D$

$T = 300K$ $\boxed{\bar{\omega}_{300K} \sim \frac{(1.3)(3)10^{-21}\,J}{6(10^{-34})\,Js} \sim 10^{13}\,s^{-1}}$

$T = 3000K$ $\bar{\omega}_{3000K} \sim 10^{14}\,s^{-1}$

$T = 10000K$ $\bar{\omega}_{10^4K} \sim 3(10^{14})\,s^{-1}$

$n_{max}(T)$ = n ass'd w/ ω_{max}

Equipartition thm.

3

$\boxed{n_{max}\, \hbar\omega_{min} \sim k_B T}$

$(\omega_{min}) \; \lambda \sim L$

$n_{max,\,300K} \sim \dfrac{10^{-21}\,J}{10^{-34}(s)(10^{-5})\,J}$

3a

$\sim \boxed{10^8}$

$n_{max,\,3000K} \sim \boxed{10^9}$

$n_{max,\,3K} \sim \boxed{10^6}$

$n_{max,\,0.003K} \sim 10^3$

$\Rightarrow$ Lots of sample-scale thermoacoustic waves

4

$n_{min}(T) = n$ ass'd ω_{max}

$\boxed{n_{min}\, \hbar\, \omega_{max} \sim k_B T}$

$\omega_{max} \sim \lambda \sim 2a_0$

4a

$n_{min,\,300K} \sim \underline{10}$

$n_{min,\,3000K} \sim 10^2$

n_{min}

$\rightarrow$ Few atom scale thermo acoustic waves

2

B) Now ω_j's fixed

debye

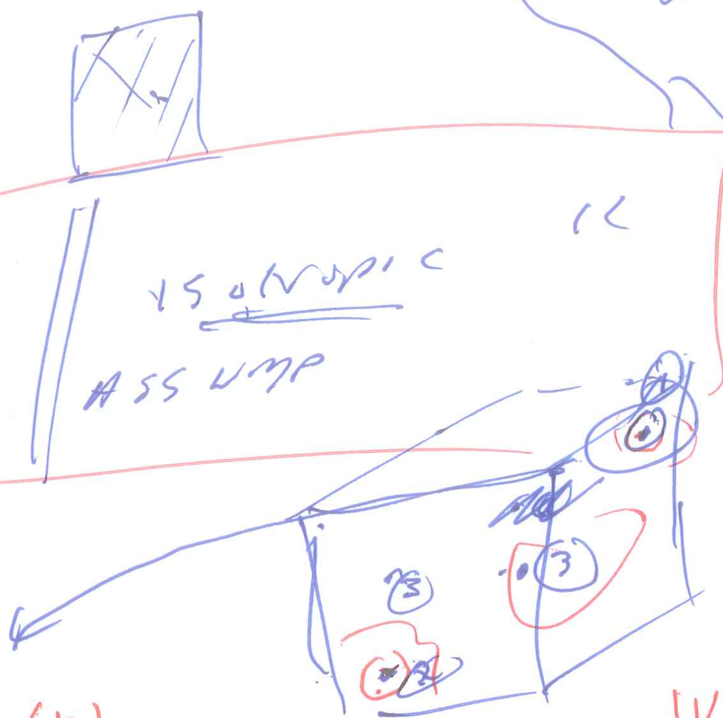
number ~~density~~ of phonon freq's, ω, in ω, $\omega + d\omega$ in $\#$ $= g(\omega)\,d\omega$

III Q2

k

isotropic

Assume

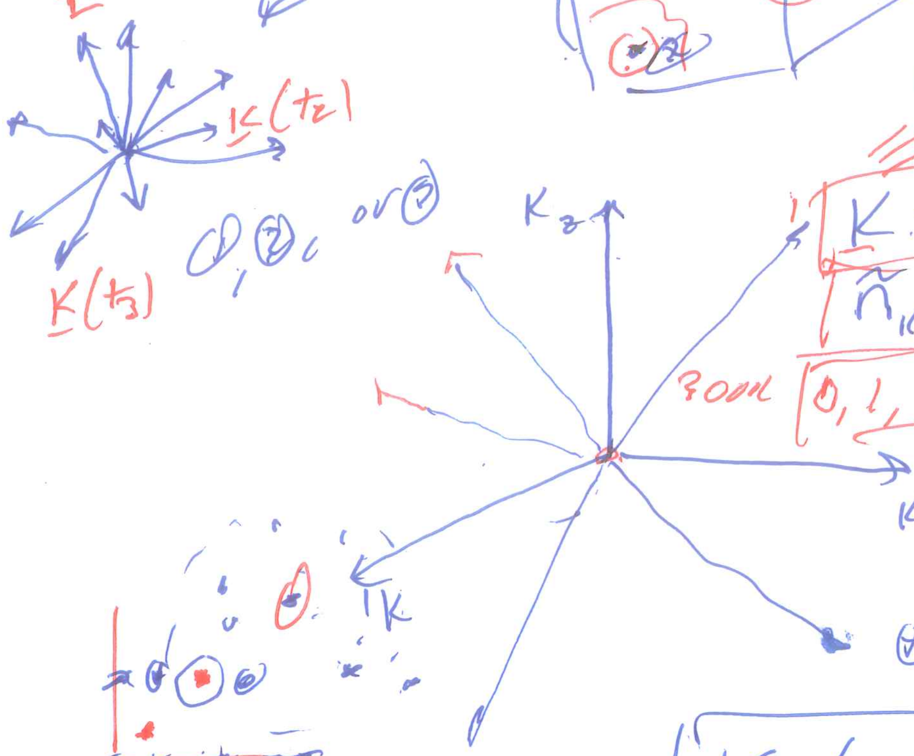


$K(t_1)$

$K(t_2)$

$K(t_3)$

(1), (2), or (3)



$K \sim K_{max} \sim \frac{2\pi}{a_0}$

$\tilde{n}_{K_{max}} \sim 10 - 10^3$

300K

0, 1, 2, 3, 4, 5 ... ~10

(4) isotropy question

(4) $\hbar\omega$ high

Isotropy assumes good for high K part of spectrum

Rudf ch10
Hill ch 5?

$\boxed{3N}$

(3)

(8) $\int_0^{\omega_D} g(\omega)d\omega = 3N$

No of phonons in w/ ω: $[\omega, \omega+d\omega]$

$C = \frac{\omega}{k}$

⊕ $K \sim K_{min} \sim \frac{2\pi}{L_{sample}}$

⊕ $n_{K_{small}} >> 1$

⊕ $\hbar\omega \sim \hbar\omega_{min}$ small energy

for any $K_s \Leftarrow \omega_{small}/c$

⊕ $\boxed{0 \leq n \leq 10^8}$

~ isotropy assumed

⇒ debye predictions of C_V solids (T)

(2) $\boxed{\hbar\omega_D = k_B T_D}$

(1) $T < T_{Debye}$ ⟸ ⊕ Good at "Low T"

$T > T_{Debye}$ ⊕ " " "HIGH T"

T_D