HW # 9

① FOR A MONATOMIC LINEAR CHAIN,

Ⓐ

$$\omega = \sqrt{\frac{4C}{M}} \left| \sin \frac{ka}{2} \right|$$

IN 1-D, THE DENSITY OF MODES IS:

$$D(\omega) = 2 \cdot \left(\frac{L}{2\pi}\right) \left|\frac{dk}{d\omega}\right|$$

+ AND − k SOLUTION

NOW $L = Na$ ← DISTANCE BETWEEN ATOMS

↑ # OF ATOMS

AND FOR $k > 0$,

$$\frac{d\omega}{dk} = \sqrt{\frac{4C}{M}} \frac{a}{2} \cos \frac{ka}{2}$$

$$= \frac{a}{2} \sqrt{\frac{4C}{M}} \left(\sqrt{1 - \sin^2 \frac{ka}{2}} \right)$$

NOW ω_m OCCURS FOR $k = \frac{\pi}{a}$ AND $\omega_m = \sqrt{\frac{4C}{M}}$

SO THAT

$$\frac{d\omega}{dk} = \frac{a}{2} \sqrt{\omega_m^2 - \omega^2}$$

AND $$\boxed{D(\omega) = \frac{2N}{\pi} \frac{1}{(\omega_m^2 - \omega^2)^{\frac{1}{2}}}}$$

Ⓑ FOR

$$\omega(k) = \omega_0 - A k^2$$

THEN $$\frac{\partial \omega}{\partial k} = -2Ak$$

BUT $$k = \begin{cases} \left(\frac{\omega_0 - \omega}{A}\right)^{\frac{1}{2}} & \text{FOR } \omega < \omega_0 \\ \text{UNDEFINED OTHERWISE} \end{cases}$$

AND

$$D(\omega) = \left(\frac{L}{2\pi}\right)^3 \frac{4\pi k^2}{\left|\frac{dk}{d\omega}\right|} = \left(\frac{L}{2\pi}\right)^3 \frac{2\pi}{A} k$$

+

AND

$$D(\omega) = \begin{cases} \left(\frac{L}{2\pi}\right)^3 \frac{2\pi}{A^{3/2}} (\omega_0 - \omega)^{\frac{1}{2}} & \text{FOR } \omega < \omega_0 \\ 0 & \text{OTHERWISE} \end{cases}$$

② THE BULK MODULUS IS DEFINED TO BE:

$$B = -V \frac{\partial P}{\partial V}$$ WHERE P IS THE PRESSURE

(SORRY, THIS IN KITTEL'S 5TH EDITION BUT NOT THE 2ND EDITION).

NOW $dU = -p\,dV + T\,ds$

AND

$$P = -\left.\frac{dU}{dV}\right|_s$$

SO

$$B = +V_0 \frac{\partial^2 U}{\partial V^2}$$

THUS THE BULK MODULUS IS A MEASURE OF HOW MUCH ENERGY IS REQUIRED TO DEFORM THE CRYSTAL.

THUS, FOR A GIVEN CHANGE IN VOLUME, ΔV (SMALL COMPARED TO V_0)

$$B \frac{\Delta V}{V_0} = \frac{dU}{dV}$$

OR THE CHANGE IN POTENTIAL ENERGY IS

$$dU = \frac{B \Delta V}{V_0} dV = \frac{B \Delta V}{V_0} d(\Delta V$$

OR

$$U = \frac{1}{2} \frac{B(\Delta V)^2}{V_0}$$

SO ENERGY DENSITY IS

$$\frac{U}{V} = \frac{1}{2} B \left(\frac{\Delta V}{V_0}\right)^2 = \frac{1}{2} B \delta^2$$ (EQ. 3.53)

BODY CENTERED

(Na IS CUBIC)

FOR A UNIT CELL, THE VOLUME IS $\frac{1}{2}a^3$ SO

$$U = \frac{1}{2} \beta \left(\frac{\Delta V}{V}\right)^2 \frac{1}{2} a^3$$

NOW EQUATING

$$U \approx \frac{1}{2} kT$$

NOTE THIS IS $\frac{1}{2} k_B T$ NOT $k_B T$. IT IS POTENTIAL ENERGY OF DISTORTION)

(NOT $\frac{3}{2} kT$ — THE OTHER kT GOES INTO SHEAR MODES)

(VALID SINCE $kT >> \hbar\omega_0$)

$$\frac{1}{2} \beta \left(\frac{\Delta V}{V}\right)^2 \frac{a^3}{2} \approx \frac{1}{2} kT$$

$$\Rightarrow \frac{\Delta V}{V} \approx \left(\frac{kT}{\beta \frac{a^3}{2}}\right)^{\frac{1}{2}}$$

WITH $a \approx 4.29 \times 10^{-8}$ cm

$kT \approx 25$ meV $= 4.14 \times 10^{-14}$ erg

AND $\beta = 7 \times 10^{10}$ erg/cm^3

WE FIND

$$\boxed{\frac{\Delta V}{V} \approx 0.123}$$

SINCE

$$V \sim a^3$$

$$\frac{dV}{V} \approx \frac{3a^2\,da}{a^3} = \frac{3\,da}{a}$$

SO $\frac{\Delta V}{V} = \frac{3\,\Delta a}{a} \Rightarrow$

$$\boxed{\frac{\Delta a}{a} \approx 0.04}$$

(4) FOR A 2-D SYSTEM,

(A) $$D(\omega) = \left(\frac{L}{2\pi}\right)^2 2\pi k \frac{dk}{d\omega}$$

IN THE DEBYE APPROX.,

$\omega(k) = V_s k$ SO

$\frac{\partial k}{\partial \omega} = \frac{1}{V_s}$. ONE IMPOSES A "CUTOFF" ON THE DENSITY OF STATES DEFINED BY:

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

SO THE DENSITY OF MODES IS:

$$D(\omega) = \begin{cases} \frac{A}{2\pi} \frac{\omega}{V_s^2} & \omega < \omega_D \\ \text{(WHERE } A = L^2) & \\ 0 & \omega > \omega_D \end{cases}$$

THE TOTAL ENERGY IS NOW

$$U = 2 \int_0^{\omega_D} d\omega \, \frac{A}{2\pi V_s^2} \hbar (\omega)^2 \frac{1}{e^{\beta\hbar\omega} - 1}$$

POLARIZATION TYPES

CHANGING VARIABLES $x = \beta\hbar\omega$, WE SEE

$$U = \frac{2A}{2\pi} \frac{(kT)^3}{V_s^2 \hbar^2} \int_0^{\frac{\Theta_D}{T}} dx \frac{x^2}{e^x - 1}$$

IN THE LIMIT $T \to 0$, $\frac{\Theta_D}{T} \to \infty$ AND

$$U \approx \frac{2A}{2\pi V_s^2 \hbar^2} (kT)^3 \underbrace{\int_0^\infty dx \frac{x^2}{e^x - 1}}_{\text{NUMBER IND. OF } T!}$$

SO THAT

$U \sim T^3$. SINCE

$C = \frac{dU}{dT}$ WE SEE THAT

$$\boxed{C \propto T^2}$$