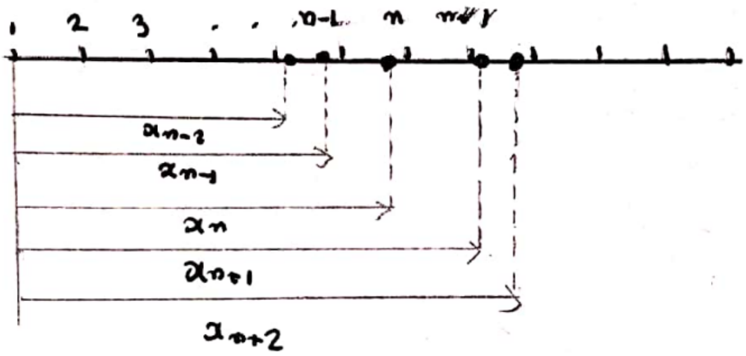
(23) (1)



Denote the position of the atom associated with lattice site n, relative to site 1, by x_n

Then the force on the atom associated with lattice site is

$$\sum_{p>0} C_p (x_{n+p} - x_n) - \sum_{p>0} C_p (x_n - x_{n-p})$$

$$= \sum_{p>0} C_p (x_{n+p} + x_{n-p} - 2x_n)$$

$\therefore$ Newtons 2^{ND} law gives

$$M\ddot{x}_n = \sum_{p>0} C_p (x_{n+p} + x_{n-p} - 2x_n)$$

Try a solution of the form

$$x_n = \varepsilon e^{-i\omega t + iKan}$$

$$\Rightarrow \quad -\omega^2 M \varepsilon e^{-i\omega t + iKan} = \sum_{p>0} C_p \left(e^{iKap} + e^{-iKap} - 2\right) \times \varepsilon e^{-i\omega t + iKan}$$

$$\Rightarrow \quad -\omega^2 M = \sum_{p>0} C_p \left(e^{iKap} - e^{-iKap} - 2\right)$$

$$= 2 \sum_{p>0} C_p (\cos Kap - 1)$$

$$\Rightarrow \quad M\omega^2 = 2 \sum_{p>0} C_p (1 - \cos Kap) = 4 \sum_{p>0} C_p \sin^2\left(\frac{Kap}{2}\right)$$

(2)

$$\therefore \quad \omega^2 = \frac{4}{M} \sum_p c_p \sin^2\left(p\frac{ka}{2}\right)$$

For small $|k|$ $\sin\left(p\frac{ka}{2}\right) \approx p\frac{ka}{2}$

$$\Rightarrow \omega^2 \approx \frac{k^2a^2}{M} \sum_p p^2 c_p$$

$$\Rightarrow \omega \approx \frac{a|k|}{M} \sqrt{\sum_p p^2 c_p}$$

(sorry, typo in the question - should have been p^2, not p)

(24) From the lecture notes, the thermal (3)

energy of a vibrational mode is

$$U = \int_0^{\omega_D} \frac{D(\omega)\,\hbar\omega}{(e^{\hbar\omega/k_BT} - 1)}\, d\omega$$

(equation (24) in the lectures), with

$$D(\omega) = \frac{V}{2\pi^2}\frac{\omega^2}{v^3} \quad \text{and} \quad \omega_D = \left(6\pi^2 \frac{N}{V}\right)^{1/3} v$$

$$\Rightarrow \quad U = \frac{V}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\hbar\omega^3}{(e^{\hbar\omega/k_BT} - 1)}\, d\omega.$$

Allowing for the 3 acoustic modes in 3-dimensions gives a factor of 3

$$U = \frac{3V}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\hbar\omega^3\, d\omega}{(e^{\hbar\omega/k_BT} - 1)}.$$

(The Debye approximation is only valid for acoustic modes).

The heat capacity is

$$C_V = \left.\frac{\partial U}{\partial T}\right|_V = \frac{3V}{(2\pi^2 v^3)} \int_0^{\omega_D} \frac{(-\hbar\omega^3)}{(e^{\hbar\omega/k_BT} - 1)^2} \left(-\frac{\hbar\omega}{k_BT^2}\right) d\omega$$

$$= \frac{3V\hbar^{-2}}{2\pi^2 v^3 k_B T^2} \int_0^{\omega_D} \frac{\hbar^4\omega^4}{(e^{\hbar\omega/k_BT} - 1)^2}\, d\omega$$

(4)

make the substitution $\omega = \frac{k_B T x}{\hbar}$, $d\omega = \frac{k_B T}{\hbar} dx$

$$\Rightarrow C_v = \frac{3V}{2\pi^2 v^3} \frac{k_B^4 T^3}{\hbar^3} \int_0^{x_D} \frac{x^4 \, dx}{(e^x - 1)^2}$$

with $x_D = \frac{\hbar \omega_D}{k_B T} = \frac{\Theta_D}{T}$, since $\Theta_D = \frac{\hbar \omega_D}{k_B} = \frac{\hbar v}{k_B}\left(6\pi^2 \frac{N}{V}\right)^{1/3}$

$$\Theta_D^3 = \frac{\hbar^3 v^3}{k_B^3}\left(6\pi^2 \frac{N}{V}\right)$$

$$\Rightarrow C_v = 9 N k_B \left(\frac{T}{\Theta_D}\right)^3 \int_0^{x_D} \frac{x^4 dx}{(e^x - 1)^2}$$

$$= 9 N k_B \left(\frac{T}{\Theta_D}\right)^3 \int_0^{\frac{\hbar \omega_D}{k_B T}} \frac{x^4 dx}{(e^x - 1)^2}$$

5)

(25) The first term is the thermal energy calculated in question (24) (in the low temperature limit). We need to calculate

$$3\hbar \int_0^{\omega_{max}} \frac{\omega}{2} D(\omega)\, d\omega.$$

In the Debye approximation $D(\omega) = \frac{V}{2\pi^2}\frac{\omega^2}{v^3}$

and $\omega_{MAX} = \omega_D = \left(6\pi^2 \frac{\mathcal{N}}{V}\right)^{1/3} v$. The factor of 3 is for the three acoustic modes.

$$3\hbar \int_0^{\omega_D} \frac{\omega}{2}\left(\frac{V}{2\pi^2}\frac{\omega^2}{v^3}\right) d\omega$$

$$= \frac{3V\hbar}{4\pi^2 v^3}\int_0^{\omega_D} \omega^3\, d\omega = \frac{3V\hbar}{16\pi^2 v^3}\,\omega_D^4$$

$$= \frac{3V\hbar}{16\pi^2 v^3}\cdot v^4 \cdot \left(6\pi^2 \frac{\mathcal{N}}{V}\right)^{4/3}$$

$$= 3\hbar v \frac{\mathcal{N}^{4/3}}{V^{1/3}} \cdot \frac{(6\pi^2)^{4/3}}{16\pi^2}$$

$$= 3\hbar v \left(\frac{3\mathcal{N}}{4}\right)^{4/3}\left(\frac{\pi^2}{V}\right)^{1/3}$$

$V = \mathcal{N} a^3$, the number of primitive cells times the volume, a^3, of a primitive cell in a simple cubic crystal. With $a = \sqrt{\frac{\Pi}{C}} \cdot v$

$$v = \sqrt{\frac{C}{M}}\left(\frac{V}{\mathcal{N}}\right)^{1/3}$$

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and

$$U = \frac{\pi^2 V (k_B T)^4}{10 v^3 \hbar} + 3\hbar v \left(\frac{3\mathcal{N}}{4}\right)^{4/3} \left(\frac{\pi^2}{V}\right)^{1/3}$$

$$= \frac{\pi^2 (k_B T)^4}{10\hbar} \cdot \left(\frac{M}{C}\right)^{3/2} \mathcal{N} + 3\hbar \sqrt{\frac{C}{M}} \left(\frac{3}{4}\right)^{4/3} \pi^{2/3} \mathcal{N}$$

$$= \mathcal{N} \left\{ \frac{\pi^2}{10\hbar} \left(\frac{M}{C}\right)^{3/2} (k_B T)^4 + 3\hbar \left(\frac{3}{4}\right)^{4/3} \pi^{2/3} \right\}$$

$$= \frac{V}{a^3} \left\{ \frac{\pi^2}{10\hbar} \left(\frac{M}{C}\right)^{3/2} (k_B T)^4 + 3\hbar \left(\frac{3}{4}\right)^{4/3} \pi^{2/3} \right\}$$

M, C and a are all intrinsic to the material.

U is linear in V, as we would expect from thermodynamics – the thermal energy is extensive.