PHONONS

Phonons are modes of crystal lattice vibrations. They are particles just like photons, but with two differences.

(1) In a crystal of N atoms, there are 3 ways to vibrate – 2 transverse
– 1 longitudinal

$\Rightarrow$ 3N modes in total

(This is different than for photons which can have an arbitrarily high # !)

(2) There are 3 polarizations not 2.

* What is the dispersion relation?

The crystal's atoms are essentially a bunch of harmonic oscillators, to a good approximation.

For the r-th atom

there's a restoring force

$$F = -\alpha(u_{r+1} - u_r) - \alpha(u_{r-1} - u_r)$$

$$= M \frac{d^2 u_r}{dt^2}$$

This is a difference equation which has travelling wave solutions

$$u_r = e^{-i\omega t} e^{i(r)k\underset{\substack{\uparrow \\ \text{lattice spacing}}}{a}}$$

The result is

$$\omega = 2\sqrt{\frac{\alpha}{M}} \left| \sin\left(\frac{ka}{2}\right) \right|$$

which for low frequencies goes over to

$$\omega = \underset{\substack{\uparrow \\ \text{speed of sound} \, \equiv v}}{(\text{const.})} \, k \qquad \left(k = \frac{2\pi}{\lambda}\right)$$

This is the dispersion relation for massless particles !!

$\Rightarrow$ Phonons are almost like photons except

(a) 3 polarizations

(b) c is speed of sound

(c) total # phonons is capped at 3N.

Using our results for photons,
we know that

$$\sum_n \rightarrow \frac{1}{8}\int_0^{n_{max}} 4\pi n^2\,dn \times 3$$

$= \#$ of modes $= 3N$

So we need

$$\frac{3\pi}{2}\int_0^{n_{max}} n^2\,dn = 3N$$

$$\Rightarrow \frac{\pi}{2} n_{max}^3 = 3N$$

Customarily called $n_{Debye} \equiv n_D$

$$\Rightarrow \boxed{n_D = \left(\frac{6N}{\pi}\right)^{1/3}}$$

Now let's calculate the energy.

$$U = \sum_n \langle \varepsilon_n \rangle = \sum_n \frac{\hbar\omega_n}{(e^{\hbar\omega_n/\tau} - 1)}$$

$$\Rightarrow \int_0^{n_D} \frac{3\pi}{2} n^2\,dn \frac{\hbar\omega_n}{(e^{\hbar\omega_n/\tau} - 1)}$$

What is $\omega_n(n)$?

For photons, $\omega_n = nc\pi/L$. Here, $\omega_n = \frac{nv\pi}{L}$.

$$\Rightarrow U = \frac{3\pi^2 v\hbar}{2L}\int_0^{n_D} dn \frac{n^3}{e^{(\hbar c\pi/L)(n/\tau)} - 1}$$

So

$$U = \frac{3\pi^2\hbar v}{2L}\left(\frac{\tau L}{\pi\hbar v}\right)^4 \int_0^{w_D} dw \; \frac{w^3}{e^w - 1}$$

with $\quad w_D = \dfrac{\pi\hbar v n_D}{L\tau}$ (the cap of modes makes an appearance!)

Definition Debye temperature θ defined by

$$w_D = \frac{\pi\hbar v n_D}{L\tau} \equiv \frac{k_B\Theta_D}{\tau}$$

i.e. $\quad \Theta_D = \dfrac{\pi\hbar v}{k_B L}\left(\dfrac{6N}{\pi}\right)^{1/3}$

$$\boxed{\Theta_D = \left(\frac{\hbar v}{k_B}\right)\left(\frac{6\pi^2 N}{V}\right)^{1/3}} \quad \therefore \frac{1}{\Theta_D^3} = \frac{k_B^3}{\hbar^3 v^3}\frac{V}{6\pi^2 N} \quad (*)$$

We can evaluate the integral if $\tau \ll k_B\Theta_D$ because then effectively $w_D \to \infty$

Then $\quad \underset{T \ll \Theta_D}{U(T) \cong} \dfrac{3}{2}\dfrac{\pi^2}{15\hbar^3 v^3} V\tau^4 = \dfrac{\pi^2}{10\hbar^3 v^3} V k_B^4 T^4$

$$(*) \quad \Rightarrow \quad \frac{\pi^2 k_B^4 T^4}{10\hbar^3 v^3} V = \frac{\pi^2 k_B T^4}{10}\left(\frac{6\pi^2 N}{\Theta_D^3}\right)$$

$$\boxed{\underset{T \ll \Theta_D}{U} = \frac{3\pi^4}{5} N k_B T \left(\frac{T}{\Theta_D}\right)^3}$$

Heat capacity @ constant V?

$C_V = \left(\frac{\partial U}{\partial \tau}\right)_V$ in "unnatural units" ☺

$$U = \frac{3\pi^4}{5} N \frac{\tau^4}{(k_B\theta_D)^3}$$

$$\Rightarrow \left(\frac{\partial U}{\partial \tau}\right)_V = \boxed{\frac{12\pi^4 N k_B}{5}\left(\frac{\tau}{k_B\theta_D}\right)^3 = C_V}_{\tau \ll k_B\theta_D}$$

"Debye T^3 Law"

- High-temperature limit? (KK 4.11)

Suppose instead $w_D \ll 1$. Then we're interested in evaluating

$$\int_0^{w_D} dw \frac{w^3}{(e^w - 1)} \quad \text{with} \quad w_D = \frac{\pi \hbar v}{L\tau} n_D \ll 1$$

For small w, the integrand is $\approx \frac{w^3}{1+w-1} \propto w^2$

$$\Rightarrow U \approx \frac{3\pi^2 \hbar v}{2L}\left(\frac{\tau L}{\pi \hbar v}\right)^4 \frac{w_D^3}{3}$$

$$= \frac{V\tau^4}{2\pi^2(\hbar v)^3}\left(\frac{\theta_D}{T}\right)^3 = \frac{V k_B T}{2\pi^2}\frac{6\pi^2 N}{V} = 3Nk_BT$$

$$\Rightarrow \boxed{\begin{array}{c} C_V = 3Nk_B \\ \tau \gg k_B\theta_D \end{array}}$$