Debye Model for 3D - summary by Dr. Colton - Class Handout

(a) Density of states $D(\omega) = \frac{1}{(2\pi/L)^3} \cdot 4\pi k^2 \cdot \frac{1}{v}$

$$= \frac{V}{8\pi^3} \cdot 4\pi \left(\frac{\omega}{v}\right)^2 \cdot \frac{1}{v}$$

$$\boxed{D(\omega) = \frac{V}{2\pi^2 v^3} \omega^2}$$

(b) cutoff frequency

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

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

$$= \frac{V}{2\pi^2 v^3} \frac{1}{3} \omega_D^3$$

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

(c) energy

$$U = \underbrace{3}_{\#\text{ of acoustic branches}} \times \int_0^{\omega_D} D(\omega) f(\omega) \hbar\omega\, d\omega$$

$$= 3 \cdot \int_0^{\omega_D} \left(\frac{V}{2\pi^2 v^3} \omega^2\right)\left(\frac{1}{e^{\hbar\omega/kT} - 1}\right) \hbar\omega\, d\omega$$

let $x = \frac{\hbar\omega}{kT} \rightarrow \omega = \frac{kT}{\hbar} x$

$\left(x_D = \frac{\hbar\omega_D}{kT}\right)$ $\quad d\omega = \frac{kT}{\hbar} dx$

$$= 3 \int_0^{x_D} \left[\frac{V}{2\pi^2 v^3}\left(\frac{kT}{\hbar} x\right)^2\right]\left(\frac{1}{e^x - 1}\right) \hbar \left(\frac{kT}{\hbar} x\right)\left(\frac{kT}{\hbar} dx\right)$$

$$\boxed{U = \frac{3V}{2\pi^2 v^3} \frac{k^4 T^4}{\hbar^3} \int_0^{x_D} \frac{x^3}{e^x - 1} dx}$$

(d) low T : $x_D \rightarrow \infty$

$$U = \frac{3V}{2\pi^2 v^3} \frac{k^4 T^4}{\hbar^3} \underbrace{\int_0^{\infty} \frac{x^3}{e^x - 1} dx}_{\frac{\pi^4}{15}}$$

(via Mathematica)

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3D cont

(d) low T, cont.

$$U = \frac{\pi^2}{10} \frac{V}{v^3} \frac{k^4}{\hbar^3} T^4$$

$$C_v = \frac{\partial U}{\partial T} = \frac{\pi^2}{10} \frac{V}{v^3} \frac{k^4}{\hbar^3} (4T^3)$$

$$\boxed{C_v = \frac{2\pi^2}{5v^3} \frac{k^4}{\hbar^3} T^3 V}$$

(can put in terms of N and $\Theta_D = \frac{\hbar\omega_D}{k}$, if desired)

(e) high T : x = small $\rightarrow e^x - 1 \simeq (1+x) - 1 = x$

$$U = \frac{3}{2} \frac{V}{\pi^2 v^3} \frac{k^4 T^4}{\hbar^3} \underbrace{\int_0^{x_D} \frac{x^3}{x} dx}_{\frac{1}{3} x_D^3}$$

$$= \frac{1}{3} \frac{\hbar^3 \omega_D^3}{k^3 T^3}$$

$$= \frac{1}{3} \frac{\hbar^3}{k^3 T^3} \left(\frac{6\pi^2 v^3 N}{V} \right)$$

$$U = \frac{3}{2} \frac{\cancel{V}}{\pi^2 v^3} \frac{k^4 T^4}{\hbar^3} \times \left[\frac{1}{3} \frac{\hbar^3}{k^3 T^3} 6\pi^2 v^3 \frac{N}{\cancel{V}} \right]$$

$$U = 3kTN$$

$$C_v = \frac{dU}{dT} = \boxed{3kN}$$

This matches the Dulong-Petit law!

(and the equipartition theorem, given 6 degrees of freedom)