Heat Capacity of 3D Phonons in Debye Model
by Dr. Colton, Physics 581 (last updated: Fall 2020)

Actual acoustic phonon dispersion (ω vs k) typically starts off linearly and then flattens out at high k values. The Debye model is an approximation whereby the dispersion is assumed to be linear the whole way ($\omega/k = v$, a constant), at least for frequencies below the Debye frequency, ω_D, at which point the states abruptly cut off instead of continuing to the zone edge.

Here's how the calculation of heat capacity proceeds for the Debye model in 3-dimensions.

(a) Density of states in 3D

$$\mathcal{D}(\omega) = \frac{1}{\left(\frac{2\pi}{L}\right)^3} \cdot 4\pi k^2 \cdot \frac{1}{v}$$

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

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

(b) Cutoff frequency calculation

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

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

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

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

(c) Energy calculation

$$U = 3 \cdot \int_0^{\omega_D} \mathcal{D}(\omega) f(\omega) \hbar\omega\, d\omega \qquad \text{(factor of 3 from the number of acoustic branches)}$$

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

Let $x = \frac{\hbar\omega}{kT}$; then $\omega = \frac{kT}{\hbar}x$, $d\omega = \frac{kT}{\hbar}dx$
(side note: define $x_D = \frac{\hbar\omega_D}{kT}$)

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

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

(d) Heat capacity calculation, low T approximation: $x_D \to \infty$

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

integral done with Mathematica, gives $\pi^4/15$

$$U = \frac{3V}{2\pi^2 v^3}\frac{k^4T^4}{\hbar^3}\left(\frac{\pi^4}{15}\right)$$

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

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

The contribution to the heat capacity from the acoustic photons at low T! (Can put in terms of N and $\theta_D = \frac{\hbar\omega_D}{k}$ if desired.)

(e) Heat capacity calculation, high T approximation: $x_D = small$

$\to x = small \to e^x - 1 \approx (1 + x) - 1 = x$

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

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

$$U = \frac{3V}{2\pi^2 v^3}\frac{k^4T^4}{\hbar^3}\frac{1}{3}\frac{\hbar^3}{k^3T^3}\left(6\pi^2 v^3\frac{N}{V}\right)$$

$$U = 3kTN$$

$$C_V = \frac{\partial U}{\partial T}$$

$$\boxed{C_V = 3kN}$$

The contribution to the heat capacity from the acoustic phonons at high T! This matches the Dulong-Petit law (and the equipartition theorem, given 6 degrees of freedom).