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

Actual acoustic phonon dispersion (\(\omega \) 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, \(\omega_D\), 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

\[
\mathcal{D}(\omega) = \frac{1}{\left(\frac{2\pi}{L}\right)^3} \cdot 4\pi k^2 \cdot \frac{1}{v} \\
= \frac{V}{8\pi^3} \cdot 4\pi \left(\frac{\omega}{v}\right)^2 \cdot \frac{1}{v} \\
\mathcal{D}(\omega) = \frac{V}{2\pi^2 v^3} \omega^2
\]

(b) Cutoff frequency calculation

\[
N = \int_0^{\omega_D} \mathcal{D}(\omega) \, d\omega \\
= \int_0^{\omega_D} \frac{V}{2\pi^2 v^3} \omega^2 \, d\omega \\
= \frac{V}{2\pi^2 v^3} \frac{1}{3} \omega_D^3 \\
\omega_D = \left(\frac{6\pi^2 v^3 N}{V}\right)^{\frac{1}{3}}
\]

(c) Energy calculation

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

Let \(x = \frac{\hbar \omega}{kT}\); then \(\omega = \frac{kT}{\hbar} x\), \(d\omega = \frac{kT}{\hbar} dx\)

(side note: define \(x_D = \frac{\hbar \omega_D}{kT}\))

\[
U = 3 \cdot \int_0^{\omega_D} \left(\frac{V}{2\pi^2 v^3} \left(\frac{kT}{\hbar} x\right)^2\right) \left(\frac{1}{e^{x} - 1}\right) \hbar \left(\frac{kT}{\hbar} x\right) \left(\frac{kT}{\hbar} dx\right)
\]
\[
U = \frac{3V}{2\pi^2 v^3} \frac{k^4 T^4}{\hbar^3} \int_0^{x_D} \frac{x^3}{e^x - 1} \, dx
\]

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

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

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

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

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

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

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

(e) Heat capacity calculation, high \(T\) approximation: \(x_D = \text{small}\)

\[
\rightarrow x = \text{small} \rightarrow e^x - 1 \approx (1 + x) - 1 = x
\]

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

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

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

\[
U = 3kTN
\]

\[
C_V = \frac{\partial U}{\partial T}
\]

\[
[ C_V = 3kN ]
\]

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).