## Debye frequency

In general

$$3N = \int_0^\infty G(\omega)\,d\omega.$$

So in the Debye model

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

whence

$$\omega_D = c_s \sqrt[3]{\frac{6\pi^2 N}{V}}.$$

In summary,

$$G(\omega) = \begin{cases} \dfrac{9N}{\omega_D^3}\omega^2 & \text{for } \omega < \omega_D \\ 0 & \text{for } \omega > \omega_D \end{cases}$$

## Debye model energy and heat capacity

The total energy is

$$E(T,V,N) = \int_0^\infty E(\omega)G(\omega)\,d\omega$$

where $E(\omega)$ is the expected energy in a single harmonic oscillator mode of frequency $\omega$. From the "simple harmonic oscillator" problem, this is

$$E(\omega) = \hbar\omega\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega}-1}\right).$$

So, in the Debye model,

$$\begin{aligned} E(T,V,N) &= \frac{9N}{\omega_D^3}\int_0^{\omega_D} \hbar\omega\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega}-1}\right)\omega^2\,d\omega \\ &= \frac{9N}{\omega_D^3}\hbar\int_0^{\omega_D}\left(\frac{\omega^3}{2} + \frac{\omega^3}{e^{\beta\hbar\omega}-1}\right)d\omega. \end{aligned}$$

The first part of this integral is

$$\frac{9N}{\omega_D^3}\frac{\hbar}{2}\int_0^{\omega_D}\omega^3\,d\omega = \frac{9N}{\omega_D^3}\frac{\hbar}{2}\left[\frac{\omega_D^4}{4}\right] = \frac{9}{8}N\hbar\omega_D.$$

The second part is

$$\begin{aligned}
&\frac{9N}{\omega_D^3}\hbar\int_0^{\omega_D}\frac{\omega^3}{e^{\beta\hbar\omega}-1}\,d\omega \qquad [\![\ldots \text{set } t=\beta\hbar\omega \text{ and } x=x(T)=\beta\hbar\omega_D\ldots]\!] \\
=\;& \frac{9N\hbar}{\beta\hbar(\beta\hbar\omega_D)^3}\int_0^x\frac{t^3}{e^t-1}\,dt \\
=\;& \frac{9Nk_BT}{x^3}\int_0^x\frac{t^3}{e^t-1}\,dt \\
=\;& 3Nk_BTD(x),
\end{aligned}$$

where we have used the definition

$$D(x)\equiv\frac{3}{x^3}\int_0^x\frac{t^3}{e^t-1}\,dt.$$

In summary,

$$E(T,V,N)=\frac{9}{8}N\hbar\omega_D+3Nk_BTD(x) \quad \text{where} \quad x=x(T)=\frac{\hbar\omega_D}{k_BT}.$$

For the heat capacity,

$$\begin{aligned}
C_V(T,V,N) &= \left.\frac{\partial E}{\partial T}\right)_{V,N} \\
&= 3Nk_BD(x)+3Nk_BTD'(x)\frac{dx}{dT} \\
&= 3Nk_BD(x)+3Nk_BT\left[-\frac{9}{x^4}\int_0^x\frac{t^3}{e^t-1}\,dt+\frac{3}{x^3}\frac{x^3}{e^x-1}\right]\left(-\frac{\hbar\omega_D}{k_BT^2}\right) \\
&= 3Nk_BD(x)+3Nk_BT\left[-\frac{9}{x^4}\int_0^x\frac{t^3}{e^t-1}\,dt+\frac{3}{x^3}\frac{x^3}{e^x-1}\right]\left(-\frac{x}{T}\right) \\
&= 3Nk_BD(x)+3Nk_B\left[3D(x)-\frac{3x}{e^x-1}\right]
\end{aligned}$$

or, in summary,

$$C_V(T,V,N)=3Nk_B\left[4D(x)-\frac{3x}{e^x-1}\right] \quad \text{where} \quad x=x(T)=\frac{\hbar\omega_D}{k_BT}.$$