

## Debye model for density of states

- Velocity of sound is taken as constant for each polarization
- The dispersion relation

$$\omega = v k$$

$v$ : velocity of sound

The density of states is then

$$\begin{aligned} D(\omega) &= \frac{V k^2}{2\pi^2} \frac{dk}{d\omega} & \frac{dk}{d\omega} &= \frac{1}{v} & k^2 &= \frac{\omega^2}{v^2} \\ &= \frac{V \omega^2}{2\pi^2 v^3} \end{aligned}$$

$N$  primitive cells in the specimen  
# of acoustic phonon modes is  $N$

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

$$\omega_D^3 = 6\pi^2 v^3 \frac{N}{V} \quad \omega_D: \text{Debye freq.}$$

This frequency is the highest possible  
↳ this also limits the wavevectors

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

In the Debye model, we don't allow wavevectors larger than  $k_D$

The total (thermal) energy per polarization type is

$$U_p = \int_0^{\omega_D} d\omega D(\omega) \hbar\omega \langle n(\omega) \rangle$$

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

If velocity is constant for all polarization

$$U = 3U_p = \frac{3V\hbar}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\omega^3}{e^{\hbar\omega/k_B T} - 1} d\omega$$

change the variable  $x = \frac{\hbar\omega}{k_B T}$   $\omega^3 = \left(\frac{k_B T}{\hbar}\right)^3 x^3$

$dx = \frac{\hbar}{k_B T} d\omega$   $d\omega = \left(\frac{k_B T}{\hbar}\right) dx$

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

$x_D = \frac{\hbar\omega_D}{k_B T}$   $\frac{\hbar\omega_D}{k_B} = \frac{1}{T}$

$$U = \frac{3V\hbar}{2\pi^2 v^3} \left(\frac{k_B T}{\hbar}\right)^4 \int_0^{x_D} dx \frac{x^3}{e^x - 1}$$

$\theta = \frac{\hbar\omega_D}{k_B}$  : Debye's temperature

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

$\frac{1}{\omega_D^3} = \frac{V}{6\pi^2 N v^3}$   $\frac{1}{\theta^3} = \frac{k_B^3}{\hbar^3 \omega_D^3}$

$$U = 9Nk_B T \left(\frac{T}{\theta}\right)^3 \int_0^{x_D} dx \frac{x^3}{e^x - 1} \quad x_D = \frac{\theta}{T}$$

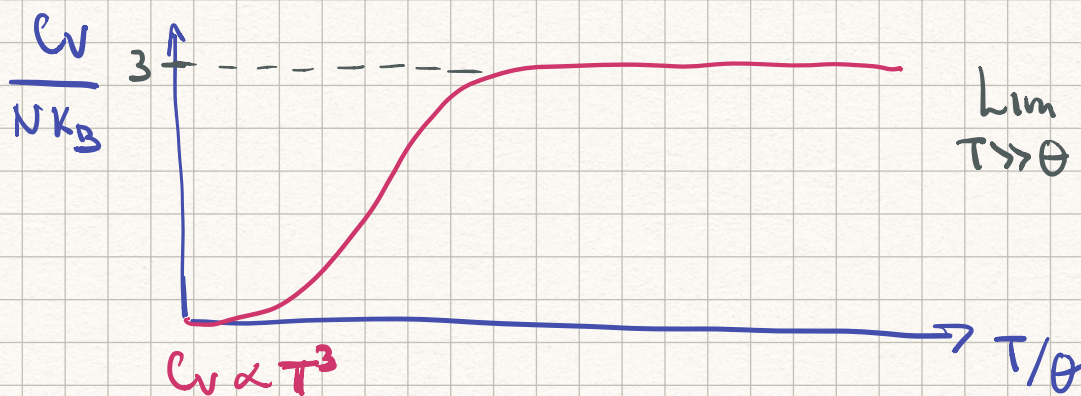
when  $N$  is the number of cells in specimen of acoustic modes

$$\begin{aligned} C_V &= \frac{\partial U}{\partial T} = \frac{\partial}{\partial T} \left( \frac{3V\hbar}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\omega^3}{e^{\hbar\omega/k_B T} - 1} d\omega \right) \\ &= \frac{3V\hbar}{2\pi^2 v^3} \int_0^{\omega_D} d\omega \omega^3 \frac{\partial}{\partial T} \left( \frac{1}{e^{\hbar\omega/k_B T} - 1} \right) \\ &= \frac{3V\hbar}{2\pi^2 v^3} \int_0^{\omega_D} d\omega \omega^3 \frac{\hbar\omega}{k_B T} \frac{e^{\hbar\omega/k_B T}}{(e^{\hbar\omega/k_B T} - 1)^2} \\ &= \frac{3V\hbar^2}{2\pi^2 v^3} \frac{1}{k_B T} \int_0^{\omega_D} d\omega \frac{\omega^4 e^{\hbar\omega/k_B T}}{(e^{\hbar\omega/k_B T} - 1)^2} \end{aligned}$$

changing variable  $x = \frac{\hbar\omega}{k_B T}$

$$C_V = 9Nk_B \left(\frac{T}{\theta}\right)^3 \int_0^{x_D} dx \frac{x^4 e^x}{(e^x - 1)^2} \quad x_D = \frac{\theta}{T}$$

$$U = 9Nk_B T \left(\frac{T}{\theta}\right)^3 \int_0^{x_D} dx \frac{x^3}{e^x - 1}$$



$$\lim_{T \gg \theta} C_V = 3Nk_B$$

Classical value of the heat capacity

## Debye $T^3$ -law

At very low temperatures  $T \ll \theta \Rightarrow x_0 \rightarrow \infty$

$$C_V = 9Nk_B \left(\frac{T}{\theta}\right)^3 \int_0^{\infty} dx \frac{x^4 e^x}{(e^x - 1)^2}$$

$$U = 9Nk_B T \left(\frac{T}{\theta}\right)^3 \int_0^{\infty} dx \frac{x^3}{e^x - 1}$$

$$\int_0^{\infty} dx \frac{x^3}{e^x - 1} = \int_0^{\infty} dx x^3 \sum_s e^{-sx} = \sum_s \int_0^{\infty} dx x^3 e^{-sx}$$

Geometric series

$$= 6 \sum_s \frac{1}{s^4} = \frac{\pi^4}{15}$$

Therefore, the energy becomes

$$U = 9Nk_B T \left(\frac{T}{\theta}\right)^3 \frac{\pi^4}{15} = \frac{\pi^4}{15} 9Nk_B \frac{T^4}{\theta^3}$$

And so 
$$C_V = \frac{\partial U}{\partial T} = \frac{4\pi^4}{15} 9Nk_B \frac{T^3}{\theta^3}$$

$$C_V = \frac{12\pi^4}{5} Nk_B \left(\frac{T}{\theta}\right)^3 \quad C_V \propto T^3$$

Debye  $T^3$ -approximation

At very low  $T$ , the  $T^3$  approx. is very good

↳ when only long wavelengths are thermally excited

$$w = \frac{v}{\lambda}$$

modes with short  $\lambda$  are too far away (in energy) to be populated at low  $T$ .

Only the modes having  $h\nu \approx k_B T$  will be excited to any appreciable extent at low  $T$

In real crystals, for the  $T^3$  approximation to hold, we usually need  $T \leq \theta/50$