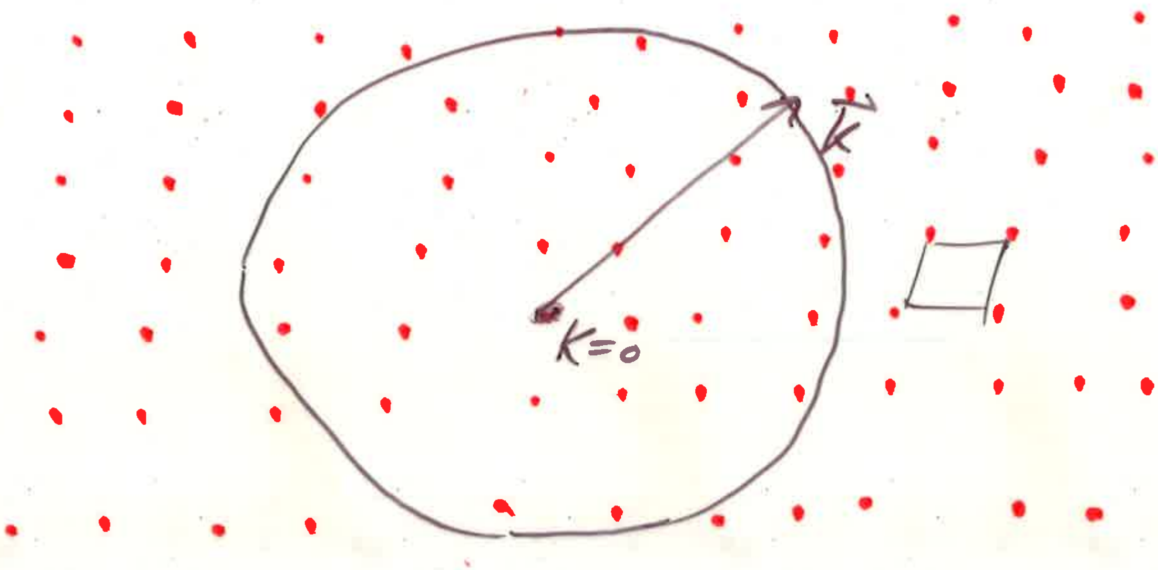
Reciprocal Lattice



$$N(k) = \pi k^2 \left(\frac{L}{2\pi}\right)^2$$

$$\frac{dN}{dk} = 2\pi k \left(\frac{L}{2\pi}\right)^2$$

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three dimensions

$$N(k) = \frac{4}{3}\pi k^3 \left(\frac{L}{2\pi}\right)^3$$

$$\frac{dN}{dk} = 4\pi k^2 \left(\frac{L}{2\pi}\right)^3$$

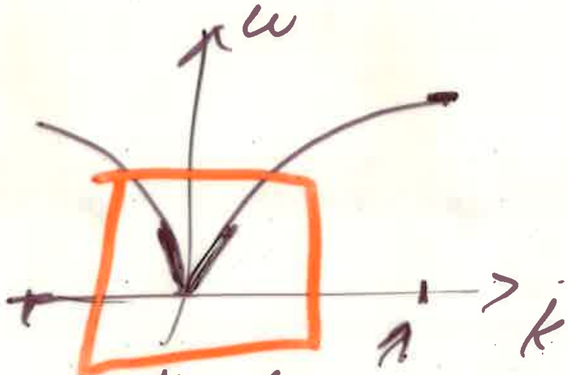
$$D(\omega) = \frac{dN}{d\omega} = \frac{dN}{dk}\frac{dk}{d\omega} = \frac{dN}{dk}\frac{1}{\left(\frac{d\omega}{dk}\right)}$$

$$= \frac{dN}{dk}\frac{1}{v_{group}} = \frac{Vk^2}{2\pi^2}\frac{1}{v_{group}}$$

Debye Model

Try to get the T^3 behavior of C_V valid at low temperature

Dispersion Relation (monatomic basis)



boundary of Brillouin Zone

Speed of phonons is constant $= v$

Debye dispersion relation
no dispersion.

$$\omega = vk$$

$$\frac{d\omega}{dk} = v$$

Density of states

$$D(\omega) = \frac{Vk^2}{2\pi^2}\frac{1}{V_{group}} = \frac{V\omega^2}{2\pi^2 v^3}$$

Constraint

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

ω_D – Debye frequency – cutoff frequency

$$\int_0^{\omega_D} \frac{V\omega^2}{2\pi^2 v^3}\, d\omega = \frac{V}{2\pi^2 v^3}\cdot\frac{1}{3}\,\omega^3\Big|_0^{\omega_D} = \frac{V\omega_D^3}{6\pi^2 v^3} = N$$

$$\omega_D = \left[6\pi^2\frac{N}{V}\right]^{1/3} v$$

Debye wavenumber $k_D = \dfrac{\omega_D}{v} = \left[\dfrac{6\pi^2 N}{V}\right]^{1/3}$

Debye Temperature : $\theta_D \equiv T_D$

$$k_B T_D = \text{energy} = \hbar\omega_D \Rightarrow T_D = \frac{\hbar\omega_D}{k_B}$$

$$T_D = \frac{\hbar v}{k_B}\left[\frac{6\pi^2 N}{V}\right]^{1/3}$$

$$U = \int \underline{D(\omega)}\ \underline{\langle n\rangle}\ \underline{\hbar\omega}\ d\omega$$

$$U_{\substack{\text{per}\\ \text{polarization}}} = \int_0^{\omega_D} \underline{\left(\frac{V\omega^2}{2\pi^2 v^3}\right)}\ \underline{\frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1}}\ \underline{\hbar\omega}\ d\omega$$

only temperature dependence

Assume v is the same for all 3 polarizations
1 longitudinal 2 transverse

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

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{3V\hbar}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\omega^3 \, d\omega \, (-1) \, e^{\frac{\hbar\omega}{k_B T}} \cdot \frac{\hbar\omega}{k_B T^2}(-1)}{\left[e^{\frac{\hbar\omega}{k_B T}} - 1\right]^2}$$

$$= \frac{3V\hbar^2}{2\pi^2 v^3 k_B T^2} \int_0^{\omega_D} \frac{\omega^4 \, e^{\frac{\hbar\omega}{k_B T}} \, d\omega}{\left[e^{\frac{\hbar\omega}{k_B T}} - 1\right]^2}$$

Low T behavior. should be $\propto T^3$ – check

$U = ?$ Define $x = \frac{\hbar\omega}{k_B T}$, $x_D = \frac{\hbar\omega_D}{k_B T} = \frac{T_D}{T}$

$= \frac{\Theta_D}{T}$

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

for low $T \ll T_D$, replace x_D by ∞

$$U = 9Nk_B T \left(\frac{T}{T_D}\right)^3 \boxed{\int_0^{\infty} \frac{x^3}{e^x - 1} \, dx} = 6\,\zeta(4)$$

$$= \frac{\pi^4}{15}$$

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{\partial}{\partial T}\left[\frac{3}{5}\frac{N k_B T^4 \pi^4}{T_D^3}\right]$$

$$= \frac{12\pi^4}{5} N k_B \left(\frac{T}{T_D}\right)^3 \leftarrow \text{Debye } T^3 \text{ Law}$$

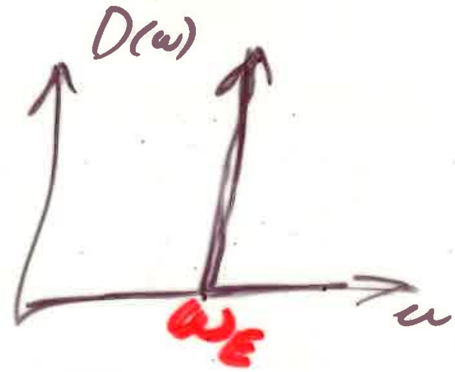
Valid for low T, also correct high T limit – Dulong-Petit Law $C_V = 3Nk_B$

Einstein Model

Independent harmonic Oscillator

one frequency ω_E

$$D(\omega) = A\,\delta(\omega - \omega_E)$$



Total # of modes $= \int D(\omega)\,d\omega = N$

$$D(\omega) = N\,\delta(\omega - \omega_E)$$

$$U = \int_0^\infty D(\omega)\langle n\rangle \hbar\omega\,d\omega = \int_0^\infty N\delta(\omega-\omega_E)\frac{\hbar\omega}{e^{\frac{\hbar\omega}{k_B T}}-1}\,d\omega$$

$$= \frac{N\hbar\omega_E}{e^{\hbar\omega_E/k_B T}-1}$$

$$U = \frac{N\hbar\omega_E}{e^{\frac{\hbar\omega_E}{k_B T}} - 1}$$

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{N\hbar\omega_E\,(-1)\,e^{\frac{\hbar\omega_E}{k_B T}}\,\frac{\hbar\omega_E}{k_B T^2}\,(-1)}{\left[e^{\frac{\hbar\omega_E}{k_B T}} - 1\right]^2}$$

$$= N k_B \left(\frac{\hbar\omega_E}{k_B T}\right)^2 \frac{e^{\frac{\hbar\omega_E}{k_B T}}}{\left[e^{\frac{\hbar\omega}{k_B T}} - 1\right]^2}$$

multiply by 3 for 3 polarization

high T limit $\quad \lim_{x\to 0} \frac{x^2 e^x}{\left[e^x - 1\right]^2} = 1$

$$C_V \to 3Nk_B \quad \text{(Dulong + Petit)}$$

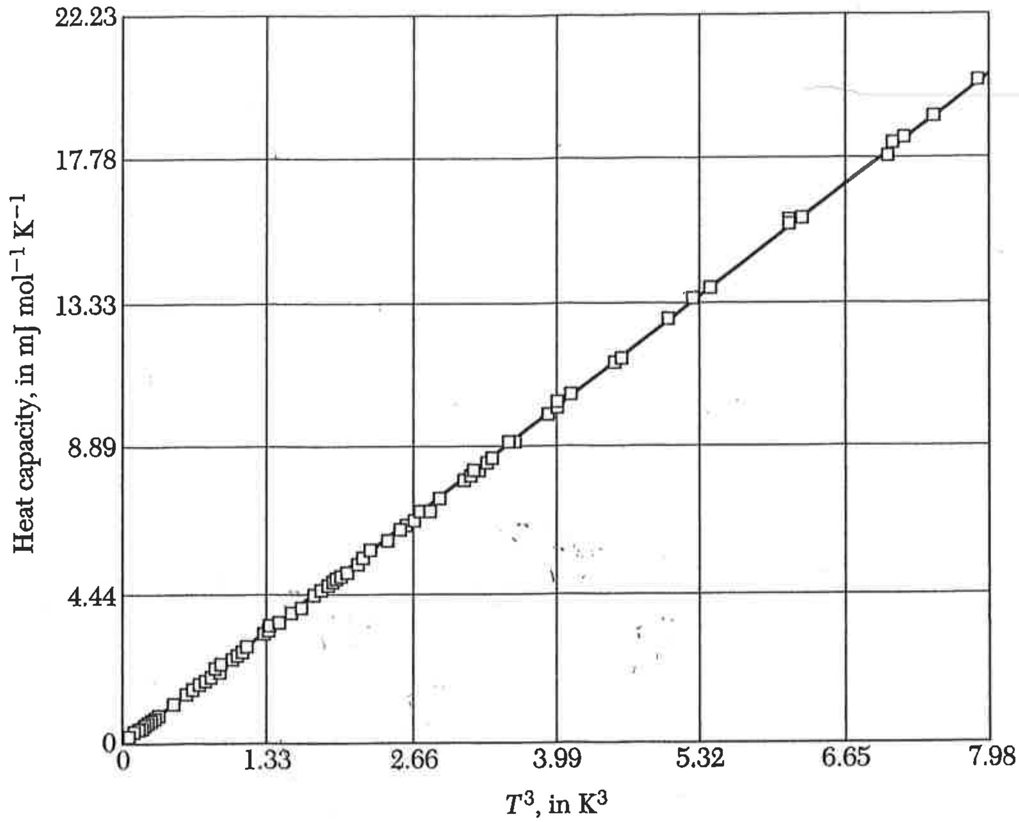


Figure 9 Low temperature heat capacity of solid argon, plotted against T^3. In this temperature region the experimental results are in excellent agreement with the Debye T^3 law with $\theta = 92.0$ K. (Courtesy of L. Finegold and N. E. Phillips.)