7.5 Debye Theory of Solids

Einstein model of solid $\rightarrow$ every atom oscillates at same frequency

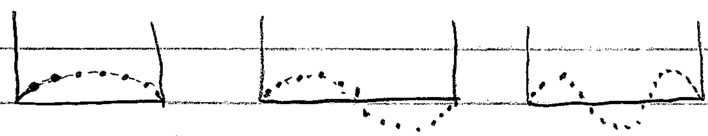
Prob 3.25 $\rightarrow$ $C_V = 3Nk_B \dfrac{(\varepsilon/k_BT)^2 e^{\varepsilon/k_BT}}{(e^{\varepsilon/k_BT}-1)^2}$

N = # of atoms, f = frequency

Big problem: Atoms don't oscillate indepently

Next level of approximation. Assume identical atoms coupled together by springs.

There are now normal modes.



These are waves. Simplification - there are 3 polarizations and they all have speed c_s

Sound waves $\overset{\text{analogy}}{\longleftrightarrow}$ Light waves

phonons $\qquad$ photons

Each mode has frequency $f = c_s/\lambda \Rightarrow \varepsilon = hf = \frac{hc_s}{\lambda}$

If you have a cube, the modes can be indexed by J_x, J_y, J_z (book uses n_x, n_y, n_z)

$\sin\left(\frac{\pi J_x}{L}x\right)\sin\left(\frac{\pi J_y}{L}y\right)\sin\left(\frac{\pi J_z}{L}z\right)$

$f = \frac{c_s}{2L}\left(J_x^2+J_y^2+J_z^2\right)^{1/2}$

As with light, the average n of a mode is for harmonic oscillator

$$\bar{n}_{Pl} = \frac{1}{e^{\varepsilon/k_BT}-1} \qquad \varepsilon = \frac{hc_s}{2L}\sqrt{J_x^2+J_y^2+J_z^2}$$

$$U = \overset{\text{polarizations}}{3}\sum_{J_xJ_yJ_z}\frac{hc_s}{2L}\left(J_x^2+J_y^2+J_z^2\right)^{1/2}\frac{1}{e^{\frac{hc_s}{2Lk_BT}(J_x^2+J_y^2+J_z^2)^{1/2}}-1}$$

For photons the j_x, j_y, j_z go from 1 to ∞.
Is this OK for phonons? Sometimes.

3 directions can vibrate

The number of modes = number of atoms $\times 3$

$$3 \frac{1}{8} 4\pi \int_0^{j_{max}} j^2 dj = N \cdot 3$$

$$\Rightarrow \frac{\pi}{2} j_{max}^3 = N \cdot 3 \Rightarrow j_{max} = \left(\frac{6N}{\pi}\right)^{1/3}$$

Convert U to an integral over $1/8$ sphere

$$U = 3 \frac{1}{8} 4\pi \int_0^{j_{max}} \frac{hc_s}{2L} j \frac{1}{e^{\frac{hc_s j}{2k_B T L}} - 1} j^2 dj$$

Convert integral to $x = \frac{hc_s j}{2k_B T L}$

$$U = \frac{3\pi}{2} (k_B T) \left(\frac{2k_B T L}{hc_s}\right)^3 \int_0^{x_{max}} \frac{x^3}{e^x - 1} dx$$

Common parameter is the Debye Temperature

$$T_D = \frac{hc_s j_{max}}{2k_B L} = \frac{hc_s}{2k_B} \left(\frac{6}{\pi}\right)^{1/3} \left(\frac{N}{L^3}\right)^{1/3} = \frac{hc_s}{2k_B} \left(\frac{6}{\pi}\frac{N}{V}\right)^{1/3}$$

$$x_{max} = \frac{T_D}{T}$$

$$\frac{3\pi}{2} k_B T^4 \left(\frac{2k_B L}{hc_s}\right)^3 = \frac{3\pi}{2} k_B T^4 \left(\frac{j_{max}}{T_D}\right)^3 = 9N k_B \frac{T^4}{T_D^3}$$

$$U = 9N k_B \frac{T^4}{T_D^3} \int_0^{T_D/T} \frac{x^3}{e^x - 1} dx$$

$T_D \simeq 90\ K$ for lead (dense and weak springs)
$T_D \simeq 1900\ K$ for diamond (light and strong springs)

If $T \gg T_D$, $x \ll 1$ in integral

equipartition

$$U = 9N k_B \frac{T^4}{T_D^3} \int_0^{T_D/T} x^2 dx = 3N k_B \frac{T^4}{T_D^3} \left(\frac{T_D}{T}\right)^3 = 3N k_B T!$$

If $T \ll T_D$, $x_{max} \gg 1$ so can replace $T_D/T \to \infty$

$$U = 9N k_B \frac{T^4}{T_D^3} \int_0^\infty \frac{x^3}{e^x - 1} dx = \frac{9\pi^4}{15} N k_B T^4 / T_D^3$$

This result is important. Remember that Einstein model has $C_V \sim \frac{1}{T^2} e^{-\varepsilon/k_B T}$. At low temp, the Debye model has much gentler dependence

$$T \ll T_D: \; C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{12}{5} \pi^4 N k_B \left(\frac{T}{T_D}\right)^3$$

The total heat capacity has contribution from electrons + from phonons

Eq 7.68 $\quad U = \frac{3}{5} N \varepsilon_F + \frac{\pi^2}{4} N k_B^2 T^2 / \varepsilon_F$

$\Rightarrow C_V = \frac{\pi^2}{2} N k_B^2 T / \varepsilon_F$

$$\frac{C_V^{metal}}{N k_B} = \left(\frac{\pi^2}{2} \frac{k_B}{\varepsilon_F}\right) T + \left(\frac{12}{5} \pi^4 \frac{1}{T_D^3}\right) T^3$$

See Fig 7.28 (pg 311)

Prob 7.57 pg 313 $\quad$ Derive C_V for any T/T_D

Easier to start from $\quad U = \frac{3\pi}{2} \int_0^{n_{max}} \frac{h c_s}{2L} n \frac{1}{e^{\frac{h c_s n}{2 k_B T L}} - 1} n^2 \, dn$

$$\left(\frac{\partial U}{\partial T}\right)_V = \frac{3\pi}{2} \int_0^{n_{max}} \left(\frac{h c_s}{2L}\right)^2 \frac{1}{k_B T^2} \frac{n^4 e^{\frac{h c_s n}{2 k_B T L}}}{\left(e^{\frac{h c_s n}{2 k_B T L}} - 1\right)^2} dn \qquad x = \frac{h c_s n}{2 k_B T L}$$

$$= \frac{3\pi}{2} k_B \left(\frac{2 k_B T L}{h c_s}\right)^3 \int_0^{x_{max}} \frac{x^4 e^x}{(e^x - 1)^2} dx$$

$$= \frac{3\pi}{2} k_B \left(\frac{T}{T_D}\right)^3 n_{max}^3 \int_0^{\frac{T_D}{T}} \frac{x^4 e^x}{(e^x - 1)^2} dx$$

$$= 9 N k_B (T/T_D)^3 \int_0^{T_D/T} x^4 e^x / (e^x - 1)^2 \, dx$$

Prob 7.59 $\quad$ Student answer

Prob 7.61
pg 313

For Liquid $\frac{C_V}{Nk_B} = \frac{1}{3}\frac{12}{5}\pi^4\left(\frac{T}{T_D}\right)^3$

$C_s = 238 \, m/s \qquad \rho = 0.145 \, g/cm^3$

$$T_D = \frac{hc_s}{2k_B}\left(\frac{6}{\pi}\frac{N}{V}\right)^{1/3}$$

$$\frac{N}{V} = \rho/m_{He} = \frac{0.145\times10^{-3}\,kg}{10^{-6}\,m^3 \quad 4\cdot1.67\times10^{-27}\,kg} = 2.17\times10^{28}\,\frac{1}{m^3}$$

$$T_D = \frac{6.626\times10^{-34}\,Js \cdot 238\,m/s}{2\cdot1.38\times10^{-23}\,J/K}\left(\frac{6}{\pi}\,2.17\times10^{28}\,m^{-3}\right)^{1/3} = 20\,K$$

$$\frac{C_V}{Nk_B} = \left(\frac{4}{5}\frac{\pi^4}{(20K)^3}\right)T^3 = 0.01\,K^{-3}\,T^3$$

almost perfect agreement

measured $\frac{C_V}{Nk_B} = \left(\frac{1}{4.67K}\right)^3 T^3 = 0.0098\,K^{-3}\,T^3$