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Quadratic Debye

Exercise 1.1 Quadratic Debye phonons (*2013 midterm pr B2*)

Assume a quadratic dispersion relation for the longitudinal and transverse modes

$$\omega = \begin{cases} b_L q^2 \\ b_T q^2 \end{cases}. \tag{1.1}$$

a. Find the density of states.
b. Find the Debye frequency.
c. In terms of $k_B \Theta = \hbar\omega_D$, and

$$\mathcal{I} = \int_0^\infty \frac{y^{5/2} e^y dy}{(e^y - 1)^2}, \tag{1.2}$$

find the specific heat for $k_B T \ll \hbar\omega_D$.
d. Find the specific heat for $k_B T \gg \hbar\omega_D$.

Answer for Exercise 1.1

Part a. Working straight from the definition

$$\begin{aligned} Z(\omega) &= \frac{V}{(2\pi)^3} \sum_{L,T} \int \frac{df_\omega}{\left|\boldsymbol{\nabla}_{\mathbf{q}} \omega\right|} \\ &= \frac{V}{(2\pi)^3} \left(\left. \frac{4\pi q^2}{2 b_L q} \right|_L + \left. \frac{2 \times 4\pi q^2}{2 b_T q} \right|_T \right) \\ &= \frac{V}{4\pi^2} \left(\frac{q_L}{b_L} + \frac{2 q_T}{b_T} \right). \end{aligned} \tag{1.3}$$

With $q_L = \sqrt{\omega/b_L}$ and $q_T = \sqrt{\omega/b_T}$, this is

$$Z(\omega) = \frac{V}{4\pi^2} \left(\frac{1}{b_L^{3/2}} + \frac{2}{b_T^{3/2}} \right) \sqrt{\omega} \tag{1.4}$$

Part b. The Debye frequency was given implicitly by

$$\int_0^{\omega_D} Z(\omega) d\omega = 3rN, \tag{1.5}$$

which gives

$$\begin{aligned} 3rN &= \frac{2}{3} \frac{V}{4\pi^2} \left(\frac{1}{b_L^{3/2}} + \frac{2}{b_T^{3/2}} \right) \omega_D^{3/2} \\ &= \frac{V}{6\pi^2} \left(\frac{1}{b_L^{3/2}} + \frac{2}{b_T^{3/2}} \right) \omega_D^{3/2} \end{aligned} \tag{1.6}$$

Part c. Assuming a Bose distribution and ignoring the zero point energy, which has no temperature dependence, the specific heat, the temperature derivative of the energy density, is

$$\begin{aligned} C_V &= \frac{d}{dT} \frac{1}{V} \int Z(\omega) \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} d\omega \\ &= \frac{1}{V} \frac{d}{dT} \int Z(\omega) \frac{\hbar\omega}{\hbar\omega/k_B T + \frac{1}{2}(\hbar\omega/k_B T)^2 + \cdots} d\omega \\ &\approx \frac{1}{V} \frac{d}{dT} \int Z(\omega) k_B T d\omega \\ &= \frac{1}{V} k_B 3rN. \end{aligned} \tag{1.7}$$

Part d. First note that the density of states can be written

$$Z(\omega) = \frac{9rN}{2\omega_D^{3/2}} \omega^{1/2}, \tag{1.8}$$

for a specific heat of

$$\begin{aligned} C_V &= \frac{d}{dT} \frac{1}{V} \int_0^\infty \frac{9rN}{2\omega_D^{3/2}} \omega^{1/2} \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} d\omega \\ &= \frac{9rN}{2V\omega_D^{3/2}} \int_0^\infty d\omega \omega^{1/2} \frac{d}{dT} \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} \\ &= \frac{9rN}{2V\omega_D^{3/2}} \int_0^\infty d\omega \omega^{1/2} \frac{-\hbar\omega}{\left(e^{\hbar\omega/k_B T} - 1\right)^2} e^{\hbar\omega/k_B T} \hbar\omega/k_B \left(-\frac{1}{T^2} \right) \\ &= \frac{9rNk_B}{2V\omega_D^{3/2}} \left(\frac{k_B T}{\hbar} \right)^{3/2} \int_0^\infty d\frac{\hbar\omega}{k_B T} \left(\frac{\hbar\omega}{k_B T} \right)^{1/2} \frac{1}{\left(e^{\hbar\omega/k_B T} - 1\right)^2} e^{\hbar\omega/k_B T} \left(\frac{\hbar\omega}{k_B T} \right)^2 \\ &= \frac{9rNk_B}{2V\omega_D^{3/2}} \left(\frac{k_B T}{\hbar} \right)^{3/2} \int_0^\infty dy \frac{y^{5/2} e^y}{(e^y - 1)^2} \\ &= \frac{9rNk_B}{2V} \left(\frac{T}{\Theta} \right)^{3/2} \mathcal{I}. \end{aligned} \tag{1.9}$$