Modern Physics

Winter Semester 23/24

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Exercise 13

§ Solids §

Problem 1: Phonon heat capacity - Debye model

The specific heat at constant volume C_v is defined as:

$$C_v = \left(\frac{\partial U}{\partial T}\right)_V . \tag{1.1}$$

The internal energy U can be expressed using the following integral:

$$U = \int_0^\infty \frac{\hbar\omega}{e^{\frac{\hbar\omega}{k_B T}} - 1} D(\omega)\, d\omega, \tag{1.2}$$

where $D(\omega)$ is the density of phonon modes. In Debye's model for the phonon contribution to the heat capacity of solids it is assumed that at low temperature acoustic modes dominate and hence $\omega = cq$ with the speed of sound c is valid. Furthermore, the total number of modes is limited to $3N$ the classical expectation for N oscillators in three dimensions:

$$\int_0^{\omega_D} D(\omega)\, d\omega = 3N, \tag{1.3}$$

where ω_D is the material dependent Debye frequency. Finally, the number of phonon modes N is assumed to be the number of allowed values $\vec{q}$ in q-space within the volume of a sphere of radius q_{max} (spherical 1^{st}-Brillouin zone):

$$N = \frac{V}{(2\pi)^3} \frac{4\pi q_{max}^3}{3}. \tag{1.4}$$

a) Find $D(\omega)$.

b) Show that the specific heat capacity of the Debye model is:

$$C_V = \frac{3 V \hbar^2}{2\pi^2 c^3 k_B T^2} \int_0^\infty \frac{\omega^4 e^{\frac{\hbar\omega}{k_B T}}}{\left(e^{\frac{\hbar\omega}{k_B T}} - 1\right)^2} d\omega. \tag{1.5}$$

c) At low temperatures only q-modes with frequencies very much smaller than ω_D are thermally excited so that the limit of the integral can be extended to infinity. Show that in the low-temperature limit $C_V \propto T^3$.
Hint:

$$\int_0^\infty \frac{x^4 e^x}{(e^x - 1)^2} dx = \frac{4\pi^4}{15}. \tag{1.6}$$

d) Using the normalization condition for the mode density given above find the cut-off frequency of the Debye model and the associated Debye temperatur $T_D = \frac{\hbar\omega_D}{k_B}$.

e) The following table gives experimental data points for the heat capacity C_V of solid argon at low temperatures. Estimate the Debye temperature of argon.

T [K]	0.4978	0.6896	1.0376	1.4059	2.0727
C_V [J K^{-1} mol^{-1}]	3.08×10^{-4}	8.13×10^{-4}	2.83×10^{-3}	6.97×10^{-3}	2.29×10^{-2}