[tex83] **Vibrational heat capacity of a solid**

The vibrational Helmholtz free energy of a harmonic crystal of N atoms in thermal equilibrium at temperature T is

$$A = \frac{1}{2}\sum_{i=1}^{3N} \hbar\omega_i + k_B T \sum_{i=1}^{3N} \ln\left(1 - e^{-\beta\hbar\omega_i}\right),$$

where the ω_i are the normal modes of transverse and longitudinal lattice vibrations (phonons). In Debye's theory, the density of modes is approximated by the functions $n(\omega) = 9N\omega^2/\omega_D^3$, where the Debye frequency ω_D is an undetermined parameter.

(a) Show that the internal energy $U = A + TS$ in the Debye approximation reads

$$U = \frac{9}{8}N\hbar\omega_D + 9Nk_B T\left(\frac{T}{\Theta_D}\right)^3 \int_0^{\Theta_D/T} dx \frac{x^3}{e^x - 1},$$

where $\Theta_D = \hbar\omega_D/k_B$ is called the Debye temperature.

(b) Derive an expression for the heat capacity $C = (\partial U/\partial T)_N$.

(c) At low temperatures the upper boundary Θ_D/T in the above integral may be replaced by infinity, $\int_0^\infty dx\, x^3/(e^x - 1) = \pi^4/15$. Use this fact to determine the leading low-temperature term of the heat capacity C.