[tex199] Heat capacity of gas due to internal degree of freedom

A classical ideal gas consists of particles with an internal degree of freedom which has the following energy-level spectrum:

$$E_{nm} = n\epsilon, \quad \epsilon > 0, \quad n = 0, 1, 2, \ldots, \quad m = 0, 1, \ldots, n. \tag{1}$$

The associated one-particle canonical partition function can thus be expressed as

$$Z = \sum_{n=0}^{\infty} (n+1) e^{-n\Theta/T}, \quad k_B\Theta = \epsilon. \tag{2}$$

The goal of this exercise is to calculate the contribution of this internal degree of freedom to the heat capacity per particle $C(T)$ of the gas by using three different and independent approaches. In each approach, $C(T)$ is inferred from Z via Helmholtz free energy $A(T)$ and entropy $S(T)$. All results are functions of Θ/T.

(a) From the first two terms of (2) (representing the lowest two energy levels) determine the leading term of the heat capacity at low temperatures.

(b) The high-temperature limit of $C(T)$ is determined by the integral term alone of the Euler-McLaurin summation formula,

$$\sum_{n=0}^{\infty} f(n) = \int_0^{\infty} dx\, f(x) + \frac{1}{2} f(0) - \frac{1}{12} f'(0) + \ldots \tag{3}$$

Evaluate Z from that first term, then infer $C(T)$ and take the limit $T \to \infty$.

(c) Evaluate the sum in (2) exactly and infer from it an analytic expression of $C(T)$ valid at all temperatures.

Solution: