

[tex90] Quantum rotational heat capacity of a gas at high temperature

The rotational spectrum of two-atomic molecules consists of energy levels

$$E_{lm} = \frac{l(l+1)\hbar^2}{2I}; \quad l = 0, 1, 2, \dots; \quad m = -l, -l+1, \dots, +l.$$

(a) Use the Euler-McLaurin summation formula

$$\sum_{n=0}^{\infty} f(n) = \int_0^{\infty} dx f(x) + \frac{1}{2}f(0) - \frac{1}{12}f'(0) + \frac{1}{720}f'''(0) + \dots$$

to calculate the first three terms of a high-temperature expansion of $Z_R = \sum_{lm} e^{-\beta E_{lm}}$.

(b) Use the result of (a) to show that the first two terms in a high-temperature expansion of the rotational heat capacity read

$$C_R \simeq Nk_B \left[1 + \frac{1}{45} \left(\frac{\Theta}{T} \right)^2 + \dots \right], \quad \Theta = \frac{\hbar^2}{2Ik_B}.$$

Solution: