# Phys. 807 — Statistical Mechanics

## HW5. due Tue Oct 18 at 4 p.m. in my mailbox.

Problem:

The partition function for the rotational degrees of freedom of $N$ diatomic molecules is given by

$$\mathcal{Z} = \mathcal{Z}_m^N$$

$$\mathcal{Z}_m = \sum_l (2l+1)(2s+1)e^{-Kl(l+1)}$$

with

$$K = \beta \frac{\hbar^2}{2I}$$

where $I$ is the moment of inertia, $(2s+1)$ is the degeneracy factor corresponding to the total nuclear spin $s$ and $l$ is summed over all allowed states of the molecular system. Calculate in the limits $(a)$ and $(b)$ (see below) the contribution of the rotational degrees of freedom to the specific heat $c_v$ for one mole of one mole of para-$H_2$ and one mole of orto-$H_2$.

$a$) Low-temperature limit ($K$ large). Keep only terms $l \leq 2$ in the partition function.

$b$) High-temperature limit. Evaluate $c_V$ to the lowest finite power in $1/T$ occurring in this limit using the Euler-MacLaurin formula

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