Problem Set 5 (due 2/17)

Problem 1 (25) Calculate specific heat of N classical oscillators governed by $H = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m} + \frac{kq_i^2}{2} \right]$

Problem 2 (25) Determine the 1st correction to the equipartition value of the quantum vibrational specific heat of a diatomic molecule at high temperature.

Problem 3 (50)

The deuterium molecule (D_2) is composed of nuclei with spin $I = 1$. One can construct $9 = (2I + 1)^2$ spin wavefunctions for the composite molecule. When properly symmetrized, there are 6 symmetric (ortho), and 3 antisymmetric (para) nuclear wavefunctions.

(a) Construct an equilibrium partition function for D_2 gas.

(b) Find the high temperature ratio of ortho- to para-D_2, assuming they are in equilibrium.

(c) Show that as $T \to 0$ true equilibrium corresponds to almost pure ortho-D_2.

(d) Using the Euler-McLaren formula, determine Z_{odd} and Z_{even} at high temperatures and, hence, the first high temperature correction to the equipartition result.

(e) Noting that H and D are chemically very similar, but that D has very nearly twice the mass of H, estimate θ - the rotational characteristic temperature for D_2, given that $\theta = 86^o K$ for H_2.

(f) Discuss the source of a possible discrepancy between your results and the actual experiment on D_2.