

ASSIGNMENT 2 FOR THE COURSE ON SOFT MATTER AND STAT. MECH.

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Due Friday Oct 29, 2004

- **1. BONUS QUESTION NOT PART OF THE ASSIGNMENT: Molecular Orbitals:** A molecule has orbital states of energies ϵ_0 , $\epsilon_1/k_B = 200K$ and $\epsilon_2/k_B = 300K$, and $\epsilon_3/k_B = 400K$. Calculate the dispersion in the energy

$$\sigma \equiv \sqrt{\langle \epsilon^2 \rangle - \langle \epsilon \rangle^2}$$

if the temperature is $300K$. What is the probability of occupation of each state?

- **2. Odd States of a Harmonic Oscillator.** Calculate the probability that a harmonic oscillator of frequency ω is in a state of odd quantum number $n = 1, 3, 5, \dots$. In the limit of zero and infinite temperature what is this probability? Does this answer agree with your expectations? Why?
- **3. Interacting Spins** Three particles are arranged in the form of an equilateral triangle. The particles are distinguishable and are fixed at the corners of the triangle. Each particle has a spin s_i which can be either up ($s_i = 1$) or down ($s_i = -1$). The Hamiltonian of the system can be written as:

$$H(s_1, s_2, s_3) = \Gamma(s_1 s_2 + s_2 s_3 + s_1 s_3).$$

Here Γ is a constant. (a) How many states does this system have? (b) Draw a series of diagrams showing the configuration of the system in each state. (c) If $\Gamma < 0$ what is the lowest energy state or states? (d) If $\Gamma > 0$ what is the lowest energy state or states? (e) Calculate the partition function for this system. (f) Calculate the free energy, the average energy and the average entropy. (g) If we define the total spin as $\sigma \equiv s_1 + s_2 + s_3$ what is $\langle \sigma \rangle$? Explain how you could have got your answer without direct calculation. (h) What is the value of $\langle \sigma^2 \rangle$?