ChE 210B: Homework 1. Due January 13, 2005.

Problem 1. The Ising model is one of the most studied models in all of statistical physics. It consists of N spins on a d dimensional lattice, and each spin can be in the up state, $s_i = 1$, or the down state, $s_i = -1$. The state of the system is denoted by the state of each spin.

$$s^N \equiv \{s_1, s_2, \ldots, s_i, \ldots, s_N\} \tag{1}$$

The energy of the system is given by

$$E(s^N) = -H \sum_{i=1}^{N} s_i - \sum_{i,j=1}^{N} J_{ij} s_i s_j \tag{2}$$

where H is an external field and J_{ij} specifies the interaction energy between pairs of spins. Here, we consider the situation in which $J_{ij} = 0$ for all i, j.

In the canonical ensemble:

- Calculate the partition function $Q(T, N)$ and the Helmholtz free energy.
- Calculate the average value of spin variable s_i, or $\langle s_i \rangle$ and the fluctuation of the position from its average $\langle \delta s_i^2 \rangle = \langle (s_i - \langle s_i \rangle)^2 \rangle$. Do these quantities depend on the spin label i?

In the microcanonical ensemble:

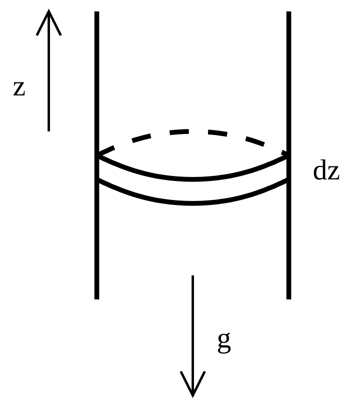
- Determine the allowed energies of the system.
- For each allowed energy E, determine $\Omega(E, N)$, the number of states with this energy.
- The answer to the previous calculation shows that $\Omega(E, N)$ is a decreasing function of E for $E > 0$; but
$$\frac{\partial \ln \Omega}{\partial E} = \frac{1}{\Omega} \frac{\partial \Omega}{\partial E} = \frac{1}{kT} \geq 0. \tag{3}$$
from thermodynamics. Explain this apparent paradox.

Problem 2. Use thermodynamics to derive the following:

$$\left.\frac{\partial E}{\partial V}\right|_{T,N} = T \left.\frac{\partial p}{\partial T}\right|_{V,N} - p. \tag{4}$$

Problem 3. Consider a long cylinder in the earth's gravitational field. The cylinder contains an ideal gas, and the gas in the cylinder at all heights is in thermal equilibrium at a temperature T. The force balance on a cross section of width dz is

$$A\Big(P_{z+dz} - P_z\Big) = -Anmgdz \tag{5}$$



where A is the area of the cross section, n is the number of molecules per unit volume. With the ideal gas law $P = nkT$, this equation becomes

$$dP = kTdn = -nmgdz \tag{6}$$

$$kT\frac{dn}{n} = -mg \tag{7}$$

and an integration implies that

$$n(z) = n(0)e^{-mgz/kT}. \tag{8}$$

The density at a height z is proportional to the exponential of the negative of the potential energy (in units of kT); this is similar to the probability of a state in the canonical ensemble. Here, provide a physical picture of what's going on in this system. Hint: understand the force balance in Eqn. 5.