Print your name clearly:_

Signature:_

"I agree to neither give nor receive aid during this quiz."

Quiz 4 for Physics 176

Professor Greenside Thursday, March 24, 2011

This 20-minute quiz is closed book and no electronic devices are allowed on your table. Please write all answers on the supplementary blank pages so that you will have plenty of space and please write your name and problem number on each supplementary page. If your answer is not reasonably readable, you will lose credit. Unless stated otherwise, you need to explain or justify your reasoning to get full credit.

Problems That Require Writing

1. (15 points) Consider a small system whose volume and energy can not change. This system is in thermodynamic equilibrium with a reservoir in such a way that the system can exchange molecules of a certain type with the reservoir. The number N_s of molecules in the system (of the given type) therefore varies with the state s of the system. The reservoir has a fixed temperature T and a fixed chemical potential μ , and the system and reservoir together form a closed system so that the total number N of molecules of the given type is conserved.

Stating clearly your assumptions and approximations, derive an expression for the probability p_s for the small system to be in a particular state s that corresponds to the system having N_s particles. Your expression will look like an "exponential of something" over a quantity \mathcal{Z} that is similar to a partition function.

2. A simple statistical physics model of the formation or unraveling of a long double-stranded biomolecule like DNA as a function of temperature is a zipper



that has a maximum of N links. The chemistry of the links is such that each link can be closed with energy 0 or open with energy $\epsilon > 0$ (i.e., it takes energy ϵ to break a link and open it). The zipper can unzip only from one side (say from the left as shown in the figure) and the *n*th link from the left can open only if all the links to the left of it (1, 2, ..., n - 1) are already open. The Nth link on the right is always closed.

- (a) (4 points) Using qualitative reasoning without mathematical calculation (but you need to explain your reasoning briefly), determine the average number of links $\langle n \rangle$ of the biomolecule in the limit of small temperatures T corresponding to $kT \ll \epsilon$.
- (b) (4 points) Using qualitative reasoning without mathematical calculation (but you need to explain your reasoning briefly), determine the average number of links $\langle n \rangle$ in the limit of large temperatures T corresponding to $kT \gg \epsilon$.

3. As a simple model of an antiferromagnet, consider four identical spin-1/2 magnetic dipoles that are placed at the vertices of a unit square:



If we consider dipole states perpendicular to the plane of the square, the state of each dipole can be described by a binary variable $s_i = \pm 1$ that has the value 1 if the dipole is up (say points in the \hat{z} direction perpendicular to the square) and has the value -1 if the dipole points down. Assuming that only nearest neighbor dipoles interact and that successive vertices are labeled 1, 2, 3, and 4 as one goes around the square, quantum mechanics suggests the following form for the energy E of this system:

$$E(s_1, s_2, s_3, s_4) = J(s_1s_2 + s_2s_3 + s_3s_4 + s_4s_1).$$
(1)

The constant J > 0, which has units of energy, is called a "coupling constant" and measures how strongly one spin couples to its neighbor. A positive J favors antiparallel nearest neighbors.

(a) (10 points) What are the different energy values E_n of this system and what are the corresponding degeneracies d_n of the distinct energy values?

Hint: there are $2^4 = 16$ possible states $\mathbf{s} = (s_1, s_2, s_3, s_4)$ since each dipole can be up or down. You can be efficient in determining all the distinct energy states by using two symmetries. First, the energy Eq. (1) does not change if all spin states are reversed, $(s_1, s_2, s_3, s_4) \rightarrow (-s_1, -s_2, -s_3, -s_4)$ since the energy depends only the relative orientation of neighboring spins. For example, a state (1, 1, 1, 1) with all spins up has the same energy E(1, 1, 1, 1) = 4J as a state with all spins down, (-1, -1, -1, -1). Second, a cyclic permutation of the spin values such as $(s_1, s_2, s_3, s_4) \rightarrow (s_2, s_3, s_4, s_1)$ can't change the energy E since, again, it is only the relative orientation of neighboring dipoles that matters. So the four states (1, 1, 1, -1), (1, 1, -1, 1), (1, -1, 1, 1), (1, -1, 1, 1), (1, -1, 1, 1), (1, -1, 1, 1), (1, -1, 1, 1), (1, -1, 1, 1).

(b) (10 points) Assuming that this small spin system is in thermodynamic equilibrium with a reservoir whose constant temperature is T, find a mathematical expression for the average energy $\langle E \rangle$ of this system as a function of temperature T, use your expression to sketch qualitatively the curve $\langle E \rangle$ versus T, and then sketch qualitatively how the heat capacity C(T) for this system varies with temperature for $T \geq 0$. (Do not waste time differentiating $\langle E \rangle$ to get C.)

The following equations may be useful:

$$S = k \ln \Omega, \qquad dU = T dS - P dV + \mu dN. \tag{2}$$

$$\beta = \frac{1}{kT}, \qquad p_s = \frac{e^{-\beta E_s}}{Z}, \qquad Z = \sum_s e^{-\beta E_s} = \sum_n d_n e^{-\beta E_n}, \qquad \langle E \rangle = \sum_s p_s E_s = -\frac{1}{Z} \frac{\partial Z}{\partial \beta}. \tag{3}$$