Homework 6: Ising Model

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1. We wrote the Hamiltonian for the 1-D Ising Model with N sites as:

$$H = \sum_{i=1}^{N}(-Js_i s_{i+1} - hs_i) = \sum_{i=1}^{N}(-Js_i s_{i+1} - \frac{h}{2}(s_i + s_{i+1})), \tag{1}$$

with $s_i \in \{+1, -1\}$. The partition function can be written

$$Z(s_1, s_2, ..., s_N) = \sum_{s_1, s_2, ..., s_N} e^{-\beta H(s_1, s_2, ..., s_N)} \tag{2}$$

Adding periodic boundaries means that $s_{N+1} = s_1$.

   (a) Write out in full the partition function with periodic boundaries for $N = 2$ (there should be 4 terms).

   (b) Show that you get the same thing using the transfer matrix formula, Tuckerman Eq. 16.6.8: $Z = \mathrm{Tr}(\mathrm{P}^{\mathrm{N}})$, where P is the transfer matrix from class (equation 16.6.6).

2. Spin Fluctuations in the Ising model

   (a) What is the formula for getting the variance of the total spin, i.e. $\chi = \mathrm{Var}(\sum_i s_i) = \langle(\sum_i s_i)^2\rangle - \langle(\sum_i s_i)\rangle^2$, from the partition function. Hint: we've done this several times before for the fluctuations of energy in the canonical ensemble, and for fluctuations of volume in NPT on the last homework.

   (b) Using this formula, compute this variance using the partition function for the 1-D Ising model with $h = 0$, in the limit of large N (i.e. you can do something like what is done in Tuckerman equations 16.6.11, 16.6.12).

   (c) Using the formula from (a), compute the variance using the mean-field partition function (Tuckerman Eq. 16.5.7, note J in the book is $2Jz$ from class)) at any h. How would you find out where χ is maximized as a function of β? (just write what you would do).

3. Lattice Gas Hamiltonian A system used for studying liquid/gas coexistence is the Lattice Gas Model. It is a lattice where every site either does or doesn't contain a molecule, which means that $n_i \in \{0, 1\}$. If two sites next to each-other are both occupied, this gives an energy of $-\epsilon$, and if a site is occupied, that gives an energy of $-\mu$.

   (a) Write the Hamiltonian and partition function for this system in 1-D (Hint: see midterm question 3)

   (b) This Hamiltonian should look a lot to you like the 1-D Ising model. Every site can have two possible states. Suppose we want to say that when a lattice site is empty, it has spin down $s_i = -1$ and when it is occupied, it has spin up $s_i = +1$. What is the formula that maps n_i to s_i?

   (c) Plugging this formula into the lattice gas Hamiltonian, what is the relationship between J and ϵ, h and μ. (Note that two Hamiltonians give the same results even if they differ by an overall addative constant).

   (d) Write the transfer matrix corresponding to the 1-d lattice gas Hamiltonian (start with the lattice gas Hamiltonian, and write what the matrix entries should be as done in Equation 16.6.4 in Tuckerman).

   (e) Find the eigenvalues for this matrix, and write the partition function for the 1-D lattice gas Hamiltonian with N sites.