

Homework 6: Ising Model

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

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

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

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

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: $Z = \text{Tr}(P^N)$, 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. $\chi = \text{Var}(\sum_i s_i) = \langle (\sum_i s_i)^2 \rangle - \langle (\sum_i s_i) \rangle^2$, 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 additive 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.