Thermal Physics: Problem Set #10

Ising Model: Mean-Field, Monte Carlo, and Exact Methods

Due: Friday April 3 by 6 pm

Reading Assignment: for Mon, Schroeder 8.2, Baierlein 16.4 (mean-field theory for Ising model)
for Wed, Baierlein 16.3-16.7 (critical exponents and universality)
for Fri, Schroeder 8.1, (diagrammatic methods for non-ideal classical gas)

Overview: This week we will continue our study of the Ising model. This simple model for ferromagnetism provides an excellent introduction to both the use of Monte Carlo methods in statistical mechanics and to the topic of mean-field theory. These approaches can be tested in detail for the Ising model since this model can be solved exactly in both 1D (which we do this week) and 2D (originally done by Lars Onsager). [The 3D Ising model has never been solved exactly.] Mean-field theory is the most widely used approach to dealing with the statistical mechanics of interacting systems. Interacting systems are difficult due to the coupling of all particles in the system via the interaction potential which results in a non-factorable (and thus, usually intractable) configurational partition function. In the mean-field approach one treats only a small subset (perhaps only one) of the particles in the system explicitly, and the effects of all other particles are taken into account in an average way (i.e., one determines the "mean-field" produced by all the other particles). One can systematically improve on mean-field theories by explicitly treating larger groups of particles. Unfortunately, this approach will *always* fail near a second order phase transition where you need to deal with very large groups of particles (and ultimately the entire system) to describe the strong fluctuation effects correctly. To deal more correctly with second order phase transitions we have another theory called the renormalization group which is discussed in the Baierlien handout.

***A1. Exact Solution for the 1D Ising Model - zero field [Super Su]**

a) Show that the exact partition function for the N-spin 1D Ising model in zero B field is given by:

$$Z(\beta,N) = [2\cosh(\beta J)]^N$$

where $\beta=1/kT$. Do this by writing out the partition function as a series of N sums over spins $s_1 \rightarrow s_N$ and noticing that the sum over s_N can immediately be done and that the result for this sum is actually independent of s_{N-1}. Now iterate the procedure, taking care with the final sum over s_1.

b) Use the above partition function to determine the internal energy E and the specific heat C_V for the 1D Ising model. Plot these functions in the form E/NJ and C_V/Nk vs $T^* = 1/\beta J$ for $0 < T^* < 5$.

A2. Mean-field theory for the Ising model: Magnetization

The mean-field result for the magnetization ($m = \langle M\rangle/N$) for the Ising model in zero magnetic field is:

$$m = \tanh(\beta J z m)$$

where z is the number of nearest neighbors on the lattice (and m is Schroeder's $\bar{s}$ and Baierleins's $\langle\sigma\rangle$). A seen in Schroeder Fig. 8.7, the condition for the possibility of spontaneous (i.e., B=0) magnetization in this approximation is that the slope (w/ respect to m) of the right hand side of the above equation exceed unity at m=0. This gives a mean-field critical temperature of $T_c = Jz/k$.

Rewrite the above magnetization equation in the form T as a function of m. Plot both the z=4 mean field result and the corresponding exact result (given last week in problem A5) for m vs $T^*=1/\beta J$ for the 2D Ising model on a square lattice.

***A3. <u>More mean-field theory for the Ising model: Specific heat</u> [Christian]**

In the mean-field approximation for the Ising model, nearest neighbor spins are assumed to be *uncorrelated* and thus the internal energy (in zero B field) is given by

$$U = -J \sum_{nn} \langle s_i\, s_j \rangle \approx -J \sum_{nn} \langle s_i \rangle \langle s_j \rangle \quad \text{(where nn refers to nearest neighbors).}$$

a) Show that the above expression reduces to $U = -JNzm^2/2$, where m is given by the self-consistent equation $m = \tanh(\beta Jzm)$ and z is the number of nearest neighbors on the lattice. (Note that I'm using m in place of Schroeder's $\bar{s}$ and Baierlein's $\langle\sigma\rangle$).

b) Use the above result to show that the mean field value for the specific heat is:

$$C_v = Nkm^2(1-m^2)/[\tau(\tau-1+m^2)] \quad \text{where } \tau = T/T_c = 1/\beta Jz.$$

c) Plot C_v/Nk vs $T^* = 1/\beta J$ using both the above mean-field expression (with z=2) and the exact expression for the 1D Ising model $[C_v/Nk = (\beta J)^2 \mathrm{sech}^2(\beta J)]$.

d) Plot C_v/Nk vs $T^* = 1/\beta J$ using both the above mean-field expression (with z=4) and the exact 2D Onsager result which, near T_c, has the form: $C_v/Nk \approx -0.4945 \log(|1-T^*/2.269|) - 0.3063$.

A4. <u>Error Estimates via Block Averaging in the 2D Ising Model</u>

When running an MC simulation one requires some way to estimate the statistical errors in one's results (i.e., generate error bars on your results!!). One way to do this is to run n independent simulations to generate a set of n estimates of the quantity of interest: $\{A_1, A_2, A_3, ... A_n\}$. (Note that A_i is the average value of A in the i-th MC run). One can then determine the mean $\langle A\rangle = (1/n)\sum_i A_i$ and variance $\sigma_A^2 = (1/n)\sum_i (A_i - \langle A\rangle)^2$ of this set of values and report a final result of $\langle A\rangle \pm \sigma_A$. In practice, this is generally done in a single long MC run. The run itself is treated as a series of "blocks" and one obtains an estimate of A for each block and then reports a final result from the mean and variance of these "block averages".

Modify the code of ising1.m or ising2.m to construct block averages for $\langle M\rangle$ and thus determine $M \pm \sigma_M$ for several temperatures both above and below T_c. (Break the run up into 5 or 10 blocks and determine the average magnetization for each block). Use the Matlab plotting command errorbar(M, sigM, 'o') to plot an array M with error bars in array sigM. Do your error bars overlap the values given by the exact expression? Investigate how Monte Carlo run length and the size of the system affect your results. (In general you can make your error bars smaller by increasing the length of the MC run but you have to be careful about interpreting what the error bars actually mean as it is possible to get "trapped" in small regions of configuration space).

A5. <u>C_v via Energy Fluctuations in the 2D Ising Model</u>

Modify the code of ising1.m or ising2.m to compute the specific heat which is given by the "fluctuation relation":

$$C_v = (1/kT^2)[\langle E^2\rangle - \langle E\rangle^2].$$

Here E is the total energy and note that you must accumulate both E and E^2 through the MC run. Determine C_v/Nk for several temperatures both above and below T_c. If you use the block averaging approach, you can compute C_v in each block and then use these block values to get a final result for C_v with an error estimate. You may also want to check how the lattice size affects your results. Compare your results with the exact expression given above in A3, part d.

A6. <u>Monte Carlo Algorithm for π</u>

Write a Matlab program that uses an accept/reject MC integration algorithm to compute π. Run your program for several different random number seeds and at least 10^5 MC steps in each case. Report a single final result with an uncertainty estimate. For at least one case, print the π estimate vs MC step.