ME 422 Statistical Mechanics for Applications

Homework 3–Monte Carlo sampling & Mean field theory

due Wednesday, October 24, 2018

1. *Nondimensional variables.* In class, we have used $\pm\epsilon$ as the interaction energy for a pair of spins. In the Matlab script IsingMarkovSee.m, I don't see any ϵ's. Nor, are there any k_B's, Boltzmann's constants. And, it is unclear what units, if any, the temperature has. What is happening here? Recall that the dynamics of a physical phenomenon as well as the steps in a MC code are governed by the non-dimensional energy, k_BT/ϵ. And, in fact, the variables in the Matlab script are not dimensional variables, but they have already been made nondimensional. For example, T in the script is the nondimensional temperature, `beta` is the nondimensional β, and `delta_E` is the nondimensional (change in) energy.

Restore the dimensions to the script's nondimensional variables. For us all to have a consistent notation, let a superscript asterisk denote a nondimensional variable. So, the variables in the Matlab script would be T^*, β^*, and ΔE^*.

(a) Express T^* in terms of dimensional variables.

(b) Express β^* in terms of dimensional variables.

(c) Express ΔE^* in terms of dimensional variables.

2. *The Metropolis acceptance criterion.* Use IsingMarkovRejections.m.

(a) For five temperatures T, find the ratio of accepted changes to attempts.

(b) What do you find as the trend in acceptances to attempts as temperature rises? Explain your finding in a few sentences.

3. *Phase change* The Matlab script IsingMarkovSee2.m is for the 2D square Ising lattice, and IsingMarkov1DSee.m is for the 1D Ising lattice. Run both programs for temperatures in the range $[1, 4]$ for `nsteps`$\geq 10^6$. Also, run both programs for a small and a large lattice: for the 2D lattice, say a small 8×8 lattice, and one as large as possible; for the 1D lattice, say a small 25 spin lattice, and one as large as possible. The objective here is to describe the behavior of the lattice as it depends on temperature.

Compared with IsingMarkov1DSee.m, the program IsingMarkovSee2.m has a few extra lines that compute `AvgMagnetization`. In order to compute `AvgMagnetization` for the 1D lattice, you will need to revise IsingMarkov1DSee.m so that it too can compute `AvgMagnetization`.

a) (i) What is being measured by `magnetization` or `magnetizationState`?
(ii) What is being measured by `AvgMagnetization`?

The visualization part of the program may be commented out when you are interested only in computing values of `AvgMagnetization`. With the extra lines to compute `AvgMagnetization`, the program will run slower, as it is now saving every magnetization state, for each nstep.

For both the 1D and 2D lattices and for the small and large lattices:

(b) Make a figure of the average magnetization as a function of temperature.

(c) Is the character of the spins at low temperature the same or different than at high temperature? Characterize the difference in terms of:

(i) The scale over which spins flip. That is, describe the size of the groups in which all spins are the same. It may be that all groups are similar in size, say, all small consisting of only several like spins. Or, groups may vary greatly in size. Describe what you see.

(ii) If there a smooth or abrupt change in behavior of the system? If abrupt, estimate the critical temperature at which the change occurs.

(iii) Describe the effect of lattice size on the distribution of spins.

4. *An example using the results from mean field theory.* The critical temperature below which iron shows spontaneous magnetization is 1043 K. Use this temperature to estimate the energy of the dipole-dipole interaction energy ϵ. Express your answer in J. And, then express your answer in terms of $k_B T_r$, where T_r is room temperature, that is, express you answer as $\alpha k_B T_r$, where α is a constant. Do you expect $\alpha > 1$?, $\alpha < 1$, $\alpha \approx 1$? Explain your answer.

You should look up the number of nearest neighbors appropriate for iron. It may be helpful to recall that chemists call the number of nearest neighbors the coordination number.