Computational Physics Project / 2D Ising Models

This project focuses on the simulation through Monte Carlo methods of 2D Ising models for magnetization. This project is similar to Exercise 10.9 in Newman.

These model a magnetic material as a 2D lattice of atoms whose magnetic moments can either be up or down. These are thermodynamic systems, so depending on the temperature, there is more or less random flipping of these moments.

Each neighboring pair of atoms (labeled i and j, where j is a neighbor in x or in y, but not along the diagonal) contributes to the total energy of the system an amount:

$$E = -Js_i s_j \tag{1}$$

Aligned moments are lower energy, therefore are the preferred state.

Since the system is thermodynamic, the spins will sometimes flip randomly. Flips that happen to be favorable happen at a constant rate, but those that are unfavorable do so at a reduced rate; reduced specifically by the Boltzman factor:

$$R = \exp\left(-\Delta E/kT\right) \tag{2}$$

We are interested in what happens to the magnetization of a system as a function of temperature. The magnetization can be defined as :

$$M = \sum_i s_i \tag{3}$$

It happens that in this case there is a simple analytic form for the magnetization as a function of temperature:

$$M(T) = \begin{cases} 0 & T > T_c \\ \frac{(1+z^2)^{1/4}(1-6z^2+z^4)^{1/8}}{\sqrt{1-z^2}} & T < T_c \end{cases} \tag{4}$$

For $kT_c \approx 2.269185J$ and $z = \exp(-2J/kT)$.

1. Prep work

- Explain in words why you should find $M \sim 0$ for sufficiently high T, and why you should find an extremal M (all spins aligned) for sufficiently low T.
- Read and briefly explain the Metropolis algorithm described in Newman section 10.3.2. We have not discussed this in class!
- Rescale the problem so that you only need one physical constant (which will be a combination of J, k, and T). Below, perform the numerical analysis in those rescaled units.

2. Writing the code

- Write a piece of code to calculate the total energy of the system (similar to part (a) of Exercise 10.9).
- Write into code the Metropolis algorithm found in section 10.3.2 of Newman. Note that you do *not* need to recalculate the full energy of the system at each trial, since most of it is unchanged (i.e. you only need the terms involving the lattice atom you picked). Use periodic boundary conditions.

3. Testing and running the code

- Now initialize your system to start with a fully magnetized (all spins aligned, with $s_i = 1$) system, at $T = 0$. Raise the temperature in small steps, and after each step run the Metropolis algorithm for long enough that the energy and magnetization seem to have converged. Use the final conditions of one temperature step as initial conditions for the next temperature step.
- Plot the magnetization and energy as a function of temperature and compare the magnetization to the analytic prediction.
- What is the physical meaning of the slope of the energy versus temperature? Can you describe in words what this slope means in terms of how much work it is to raise the temperature?
- If you add a term to E that accounts for an external magnetic field:

$$-H \sum_i s_i \tag{5}$$

  how does this change the behavior of the system when you start with $T = 0$ and raise the temperature? Try both H positive and negative.
- Try a few runs where you start with random spin orientations and $T \gg T_c$, and cool the system down. What do you notice about the final result? What if you include a non-zero H?