Computational Physics Project / 2D Ising Models

This project focuses on the simulation through Monte Carlo methods of 2D Ising models for magnetization.

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:

$$E = -J s_i s_j \tag{1}$$

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 :

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

- Explain in words why you should find $M \sim 0$ for sufficiently high T, and find an extremal M (all spins aligned) for sufficiently low T.

- Write into code the Metropolis algorithm found in Section 17.4 of Landau. 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). Think about the scaling of the problem. Does your code need to carry around J, k, and T? Use periodic boundary conditions.

- 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.

- Plot the magnetization and energy as a function of temperature. Compare to the analytic solution found in Section 17.3.1 of Landau (this will indicate to you how far up in T you need to go).

- 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:

$$-H \sum_i s_i \tag{4}$$

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?