Lab Assignment – 12 (2023)
PH-566

Q1. The Ising model is a model for ferromagnetism. Here we consider a 2-D model, involving a periodic square lattice of atoms with magnetic dipoles (spins of either +1 or −1) interacting with their 4 neighbors. Depending on the temperature of the system, they can either all align (becoming magnetic) or take on a random configuration (no magnetism).

The magnetic potential energy between two spins is proportional to their dot product as $-JS_i.S_j$ Where $J > 0$ is the interaction strength. The total energy of the system is:

$$E = -J\sum_{ij} S_i.S_j$$

where <*ij*> indicates that the sum over pairs that are adjacent on the lattice (the 4 neighbors). Model this problem using the Monte carlo (MC) method by creating a lattice of 20×20 atoms, each initially given a random spin. When computing the total energy of the system, be careful not to double count the pairs.

This energy can be used with the Metropolis algorithm, as discussed in the class. Take $J = 1$, and work in units where Boltzmann constant k_B=1. Your move set will consist of picking an atom at random and flipping its spin. Evaluate this new energy and accept the new state if it meets the Metropolis acceptance criteria,

$$P = \begin{cases} 1 & E_{New} \leq E_{Old} \\ e^{-\beta(E_{New}-E_{Old})} & E_{New} > E_{Old} \end{cases}$$

Where P is the acceptance probability. If the change is rejected, then revert the spin of the atom you changes

You will need a lot of iterations (like 10^6) to get a system that goes to equilibrium.

Start with a temperature T=1, and increase it in small steps (like $\Delta T = 0.25$) to T=3. Somewhere between T=2 and T=2.5, you will notice that the system goes from ordered (all the spins aligned) to disorder (no clear alignment).

Make a plot of the energy of the system and $|M|$ (absolute value of magnetization) as a function of T

$$M = \sum_i S_i$$

Note: You will want to make sure that your code is reasonably optimized—for a 20×20 lattice with 10^6 iterations, it may take a few minutes per temperature value.