1. Ising Model

The Ising model comprises spins S_i on a lattice, each of which can point up, $S_i = 1$, or down, $S_i = -1$. Each neighbouring pair of aligned spins lowers the energy of the system by an amount $J > 0$. Thus, given a spin configuration $\{S_i\}$, the total energy is

$$E(\{S_i\}) = -J \sum_{\langle ij \rangle} S_i S_j \tag{1}$$

where the sum is over all distinct nearest neighbour pairs $\langle ij \rangle$. According to the Boltzmann distribution, that probability of observing a given configuration $\{S_i\}$ at equilibrium is

$$P(\{S_i\}) = \exp\left[-E(\{S_i\})/(k_B T)\right] \tag{2}$$

where k_B is Boltzmanns constant and T is the temperature.

As the physics of the system is determined by the ratio between J and $k_B T$ (which enters the Boltzmann weight), we can take any two of J, k_B and T equal to unity with no loss of generality – in practice calculations normally have $J = k_B = 1$. [Of course, setting $J = k_B = T = 1$ *does* lose generality.]

1. One way to sample an equilibrium state of the Ising model is to use *Glauber dynamics* in conjunction with the Metropolis algorithm. Specifically, one chooses a site i at random, and considers the effect of flipping the spin at this site. Let the resulting change in energy if the move is actually performed be ΔE. Then, if $\Delta E \leq 0$, the spin flip is always flipped; otherwise it is flipped only with probability $\exp(-\Delta E/k_B T)$. For the coding, it is useful to write down an expression for ΔE given the choice of lattice site i. How many other spin variables enter this expression?

   Hint: There are many cancellations; make use of all of them to avoid unnecessary computations.

2. An alternative way to sample an equilibrium state of the Ising model is to use *Kawasaki dynamics*. Here, one chooses randomly two distinct sites i and j (these may also be nearest neighbours), and considers the effect of exchanging this pair of spins. Again, a decrease in energy means the exchange is then made; otherwise it is made with probability $\exp\left(-\Delta E/k_B T\right)$ where ΔE is the change in energy that would result from the exchange. Think whether this update rule sample the same equilibrium state as the Glauber dynamics? Write down an algorithm for computing E given the choice of lattice sites i and j.

   Hint: There are two ways to do this. Either (i) consider the exchange as two consecutive single spin flips, so that ΔE is the sum of the energy changes for the two moves separately; or (ii) consider the exchange as a pair of moves made simultaneously, and write down a single expression for ΔE accordingly. Extra thought may be needed in the case where i and j are nearest neighbours!

3. Write a Python program to simulate the Ising model on the two-dimensional square lattice with periodic boundary conditions (you should ideally use a 50×50 square lattice). Your program should allow the user to choose the system size, temperature and the dynamics that are used (Glauber or Kawasaki), when running the code (e.g., these may be arguments on your command line). You should also be able to show an animation of the simulation, either by using matplotlib within your code, or by interfacing it with gnuplot.

4. Describe in qualitative terms the difference between the behaviour of the system at high and low temperatures. Is this difference evident for both choices of dynamics?

5. The total magnetisation of a configuration $\{S_i\}$ is defined as $M = \sum_i S_i$. Use your program to estimate the average value of the total magnetisation in the equilibrium state, $\langle M \rangle$, and of the susceptibility

$$\chi = \frac{1}{N k_B T} \left(\langle M^2 \rangle - \langle M \rangle^2 \right). \tag{3}$$

Plot these as a function of temperature, T, and use one of the graphs to estimate the location of the critical temperature at which the system spontaneously magnetises under Glauber dynamics. [Think about why one of the two graphs is more useful than the other for an accurate determination of the critical point.]

Hint: When taking measurements (here and in what follows) we need to: (i) wait a sufficiently long equilibration time before starting recording measurements so as to lose memory of the initial condition; (ii) wait a sufficient time in between measurements to avoid them being too correlated. The first issue would introduce a systematic error, the second issue is less serious but leads to inefficiency, and renders the estimate of error more complicated (see lecture notes). A suggestion is to wait 100 sweeps for equilibrations, and 10 sweeps in between measurements – you are welcome to experiment with these values!

6. Consider now the average of the total energy, $\langle E \rangle$, and the heat capacity (per spin)

$$C = \frac{1}{N k_B T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right), \tag{4}$$

and plot these as a function of T (including errors). Use these graphs to estimate the critical temperature – you should get a very similar value with respect to the estimate using the magnetisation/susceptibility graphs.

7. Why does measuring M as a function of T not yield useful information when you switch to Kawasaki dynamics? Consider instead the total energy, E, and the heat capacity per spin. Does the choice of dynamics affect the critical temperature?