1. Ising Model

The Ising model comprises N spins S_i on a lattice (so that $i = 1, \ldots, N$), 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.]

[Following is a list of tasks/questions to guide you through the checkpoint. Whilst we hope it is useful, you will not need to write down the answers to each point explicitly. For a list of the points considered by the markers, see the Marksheet.]

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 ΔE 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. 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

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

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. In these graphs, as in all graphs in the checkpoint, we recommend to use a range for T between 1 and 3 in steps of 0.1.

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 – note you will need ideally about 10000 sweeps per temperature after equilibration (so 1000 measurements per temperature). You are welcome to experiment a bit with these values!

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

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

and plot these quantities 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.

6. 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 to find the critical temperature for Kawasaki dynamics.

3.3 Figure and datafile checklist for checkpoint

For convenience, the basic plots and datafiles which you should have for the quantitative analysis for this checkpoint are given below (these correspond to the graphs and datafiles mentioned in the marksheet).

1. For Glauber dynamics, you should have a plot of the average energy and of the average absolute value of the magnetisation, a specific heat plot and a susceptibility plot. You should also have the corresponding datafiles to check selected points quantitatively.

2. For the Kawasaki dynamics, you should have a plot of the average energy and specific heat. You should also have the corresponding datafiles.

3. For the specific heat curves and datafiles, you should also account for error bars with a resampling method (bootstrap or jacknife).