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.

1. Why we can take any two of J, k_B and T equal to unity with no loss of generality? Why do we lose generality if all three parameters are set to unity?

2. 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 $\Delta E < 0$, the spin flip is always flipped; otherwise it is flipped only with probability $\exp(-\Delta E/k_B T)$. What happens if $\Delta E = 0$? Write down an expression for ΔE given the choice of lattice site i. How many other spin variables enter into this expression?

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

3. An alternative way to sample an equilibrium state of the Ising model is to use *Kawasaki dynamics*. Here, one chooses two distinct sites i and j (not necessarily 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. Does 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 is needed in the case where i and j are neighbouring sites).

4. Write a Java program to simulate the Ising model on the two-dimensional square lattice with periodic boundary conditions. Your program should allow the user to choose the system size, temperature and the dynamics that are used. It should also be able to show a visualisation of the state of the lattice as it is running.

5. 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?

6. The total magnetisation of a configuration si 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 the susceptibility

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

   Plot these quantities as a function of temperature, T, (with errors!) to estimate the location of the critical temperature at which the system spontaneously magnetises under Glauber dynamics.

7. Why doesnt measuring M as a function of T yield useful information when you switch to Kawasaki dynamics? Consider instead the total energy, E, and the heat capacity (per particle)

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

   and plot these as a function of T. Does the choice of dynamics affect the critical temperature?

8. Start your system in a high temperature configuration, and suddenly decrease the temperature below the critical temperature. Describe the subsequent evolution of the system. What do you notice if you take T to zero?