Simulating the Ising Model on the Computer

1 The Model

The Ising Model is perhaps one of the most important models in Physics. It is a mathematical model that tries to 'explain' the origin of ferromagnetism. Ferromagnetic materials exhibit spontaneous magnetisation below a certain temperature, called the Curie temperature. Above this temperature, they behave like paramagnetic materials. The origin of ferromagnetism is complicated, but in its simplest form, it can be stripped down to the interaction between magnetic moments of atoms in a solid lattice (though that is not the complete story). The magnetic moment is quantum mechganical in origin. The magnetic moment $\vec{\mu}$ of an atom is related to its spin angular momentum $\vec{s}$ as

$$\vec{\mu} = -(g\mu_B)\vec{s} \tag{1}$$

where $\mu_B = e\hbar/2m_e$ is a fundamental unit called the *Bohr magneton* (e and m_e are the charge and mass of an electron and $\hbar = h/2\pi$ where h is Planck's constant), g is a so-called *structure factor* (which depends on the electronic configuration) and $\vec{s}$ is the spin of the atom, measured in units of $\hbar/2$. In the simplest case, the spin of the atom is due to a single unpared electron, in which case its component along any given direction (which we can denote as the z direction) takes discrete values $s_z = \pm 1$. Another simplification is that the most significance piece of interaction is between neighboring atoms, in which case the interaction energy between neighboring atoms can be written as

$$E_{\langle ij \rangle} = -\alpha \ \vec{\mu}_i \cdot \vec{\mu}_j \tag{2}$$

where $\langle\rangle$ denotes nearest neighbors and α is a parameter that determines the strength of coupling between the magnetic moments. Yet another simplification can be made in whcih we assume that something in the lattice singles out a special direction, so that the component of magnetic moment only along that direction is relevant. Denoting that direction as z, the interaction energy becomes

$$\begin{aligned} E_{\langle ij \rangle} &= -\alpha \ \mu_{iz}\mu_{jz} \\ &= -\alpha(g\mu_B)^2 s_{iz}s_{jz} \\ &= -J s_{iz}s_{jz} \end{aligned} \tag{3}$$

where J is a constant. In this stripped down version, we have the Ising Model. In brief, there is a lattice of spins, with each spin taking values (along some preferred direction) ± 1, and the interaction between mearest neighbors given by eqn.(3). It is usually customary to use the symbol σ instead of s_z. Then, the total energy of interaction of the system of spins can be written as

$$E = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \tag{4}$$

In presence of an external magnetic field, the interaction of each spin with the magnetic field can be modelled as a term of the form $-KB\sigma_i$ where B is the magnetic field (again along the preferred direction) and K is the interaction strength. Then, the total energy of the system, in presence of an external magnetic field, is

$$E = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i \tag{5}$$

where $h = KB$ is an 'effective' magnetic field (incorporating coupling strength) with dimension of energy. In this form, constants J and h have the same dimension (that of energy) and the relative effect of the spin-spin interaction and the interaction with the external field will depend on the dimensionless ratio h/J.

2 Spontaneous Magnetisation

Given an Ising ferromagnet at temperature T, the probability of the system having a spin configuration $\{\sigma_i\}$ is given by the (canonical) Boltzmann distribution

$$P\{\sigma_i\} = \frac{1}{Z} e^{-\beta E} \tag{6}$$

where $\beta = 1/k_B T$, k_B the Boltzmann constant. The magnetisation per spin for configuration $\{\sigma_i\}$ is given by

$$m\{\sigma_i\} = \frac{1}{N} \sum_i \sigma_i \tag{7}$$

where N is the total number of spins. In thermal equilibrium, the mean magnetisation is given by the average of (7) over the probability distribution (6)

$$\bar{m} = \sum_{\{\sigma_i\}} m\{\sigma_i\} P\{\sigma_i\} \tag{8}$$

where the sum is over all possible spin configuration, with each spin taking values $+1$ or -1. The system exhibits spontaneous magnetisation, if there exists a temperature T_c such that $\bar{m} \neq 0$ for $T < T_c$, with $h = 0$. To avoid boundary effects, it is useful to consider a system of spins on a lattice with periodic boundary conditions. We consider a 2D lattice, with opposide edges identified

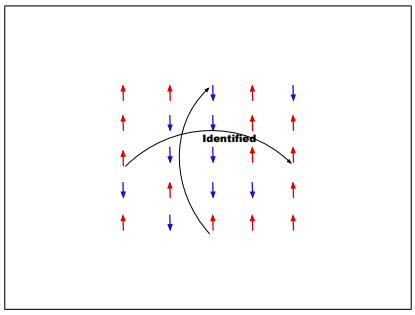

Figure 1: Spin lattice with opposite edges identified.

To explore the existence of spontaneous magnetisation, we simulate the probability distribution (6) using the *Metropolis Algorithm*). For this system, the algorithm proceeds as follows:

1. Start with a random configuration of spins and compute the magnetisation.
2. Pick a spin at random and flip it. Compute the change in energy of the system, ΔE.
3. The Metropolis acceptance probability is given by

$$P = min\left(1, e^{-\beta \Delta E}\right)$$

4. If the move is rejected, flip the spin back and compute the magnetisation.
5. If the move is accepted, keep the spin flipped and compute the magnetisation.
6. Go to step 2.

The mean magnetisation is computed by averaging over the values of magnetisation over the trials. To compute the change in energy ΔE, we just need to compute the change in interaction energy of the flipped spin. If, say the i^{th} spin is flipped, the change in energy will be

$$\Delta E = 2J\sigma_i \sum_{\langle j \rangle} \sigma_j \tag{9}$$

where the sum is over the nearest neighbors of the spin.
In calculating ΔE for a given spin flip, we need to identify the neighbors of the spin. This is achieved by constructing a 'neighbor table' for each spin. To do this, the spins are numbered as follows

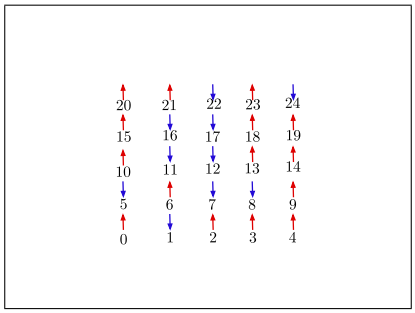

Figure 2: Spins numbered.

Then, given that the opposite edges are identified, the nearest neighbors of say spin 1 are 0, 2, 6 and 21. Similarly, the nearest neighbors of spin 5 are 0, 6, 10 and 9. The following Python program implements the Metropolis algorithm for a given temperature and graphically displays the spin configuration for that temperature