Project B4: Thermodynamic simulations using the Ising model

Key Topic; Monte Carlo methods

1 Background

Ferromagnetic materials contain domains with aligned spins even in the absence of an external magnetic field. As temperature is increased, increasing thermal fluctuations in the spins lead to demagnetisation, or "melting" of the ferromagnet. In the Ising model, the state of a system is given by a configuration of a set of spins on a lattice, each of which is either up or down. The total energy of the system is given by the interactions between interacting spins and between the spins and any external magnetic field;

$$E = -\frac{1}{2}\sum_{i,j} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j - \mu \sum_k \mathbf{S}_k \cdot \mathbf{B} \ . \tag{1}$$

where $\mathbf{S}_i$ is the spin on the i^{th} site (either 1 or -1), J the interaction energy, μ the Bohr magneton and $\mathbf{B}$ the applied magnetic field. In this project we will consider only neighbouring interactions so that $\mathbf{J}_{ij} = J$ for neighbouring sites and 0 otherwise[1]. In ferromagnetic materials ($J > 0$) alignment of spins leads to negative contributions to E and minimises the total energy. Thus, at very low temperatures T, the most favourable state has all spins aligned. At higher temperatures, thermal fluctuations allow spin flipping to occur, and domains of differently aligned spins may exist. At very high temperatures a random, fluctuating spin configuration is reached and magnetisation is lost. For K spins there are 2^K different possible states of the system, which rapidly becomes too many to include in an exact calculation. Instead, the system may be simulated by a probabilistic method, and statistical averages of relevant physical quantities found by a Monte Carlo sampling technique. The thermodynamic basis of the model is the assumption that all microscopic configurations or "microstates" of the system are possible, with a probability that depends on the energy of the state. This leads to a probability $\mathcal{P}(\alpha_j)$ of the system being in state α_j given by a Boltzmann distribution:

$$\mathcal{P}(\alpha_j) = \frac{e^{-E(\alpha_j)/k_B T}}{Z} \ , \tag{2}$$

where

$$Z = \sum_{\alpha_j} e^{-E(\alpha_j)/k_B T} \ , \tag{3}$$

k_B is Boltzmann's constant and $E(\alpha_j)$ is the energy of state α_j.

2 Project

In this project you will simulate the statistical mechanics of a 2D array of $N \times N$ spins at different temperatures using a Monte Carlo sampling method (the Metropolis algorithm). The quantities of interest are the total energy (1), the magnetisation

$$\mathbf{M} = N^{-2}\sum_k \mathbf{S}_k \ , \tag{4}$$

the specific heat capacity

$$C = N^{-2}\frac{1}{k_B T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right) \ , \tag{5}$$

and the magnetic susceptibility

$$\chi = N^{-2}\frac{J}{k_B T}\left(\langle S^2\rangle - \langle S\rangle^2\right) \ , \tag{6}$$

[1] By a neighbour we mean left/right/up/down with respect to the site under consideration. Sites on the diagonal are not considered neighbours.

where $\langle x \rangle$ represents the ensemble average of x over the different configurations of the system and $S = \sum_k \mathbf{S}_k$. First we will consider the case where $B = 0$ and study the effect of temperature on these quantities. It will make sense to define $\beta = J/k_B T$ and vary β, rather than varying J and T independently. Then the energy will be calculated in units of J.

3 Simulation of 2D array with no external field

Set up a 2D array of $N \times N$ spins and initialise the spins as aligned (if starting from low T, a "cold start") or random (if starting from high T). At subsequent temperatures it will save time to use the final configuration of the last temperature as a starting point for the next one. Then, at each temperature repeat the following steps in a loop:

- Choose one of the spins at random and calculate the change in total energy ΔE, if it were to be flipped.
- Decide whether or not to flip the spin using a Metropolis algorithm. This means that if $\Delta E < 0$ the spin should flip. If $\Delta E > 0$ then generate a random number, X, between 0 and 1 and flip the spin only if $X < \exp(-\Delta E/k_B T)$. Otherwise, leave the system unchanged.
- Update the total energy E and magnetisation M of the system.
- Continue iterating until a condition approximating to equilibrium has been reached.
- Then start taking the 'measurements' including calculation of the averages $\langle E \rangle$, $\langle E^2 \rangle$, $\langle S \rangle$, and $\langle S^2 \rangle$ that are needed to calculate C and χ.

Try with a lattice of N at least 10 and β in the range 0 to 1. You may need a larger lattice to study the phase transition more closely.

In the development of your code be aware:

- The number of iterations taken to reach the equilibrium will take longer close to a phase transition. You should build in some way of checking whether a steady state has been reached, e.g., by checking that a moving average of E is neither increasing or decreasing.
- You should apply periodic boundary conditions in both directions to avoid "end" effects. Periodic boundary conditions simply mean that we assume that the left side is connected to the right side of our array, and the top to the bottom[2].
- Don't forget to include contributions from unflipped spins in the averages. These unflipped states usually represent lower energy states and are important contributions to the average.
- You do not need to recalculate E and M completely and each step, only the change in these due to the single spin flip (if it occurred).
- You will get better statistics if you average over several simulations with different random number seeds.
- If using an interpreted language like `Python` rather than a compiled language such as `C/C++`, your code will likely run more slowly. Bear in mind that you *might* need to be on the conservative side when doing the 'production calculations', e.g., in terms of the number of iterations used for averaging at a given β. However in this case, ensure you understand how this potentially affects the results.

[2] One way to do this is to use the modulus as $(i \pm 1) \bmod N$ when calculating the index of the neighbour.

4 Results

Make plots showing how each of the thermodynamic quantities (total energy, magnetisation, specific heat capacity & magnetic susceptibility) varies with the temperature parameter. Check that the limiting values of E and M at low and high T do what you would expect. You should find that at a certain, critical temperature the magnetisation changes sharply, indicating a phase transition. Check that the other thermodynamic quantities behave appropriately at the phase transition. Discuss what is happening to the spatial pattern of the spins as T is varied and how this relates to your other observations.

5 Cooling, heating and an external magnetic field

Now introduce an external magnetic field and study the effect on the temperature dependence of M and E. Try a value of μB of around $0.5J$, aligned in either sense. Does B have any effect on the pattern of spin domains? Finally, for a fixed value of temperature, vary the external field from a large positive value (say, $\mu B = J$) to a large negative value (say, $\mu B = -J$) and back again. Discuss what is happening to the energy and magnetisation of the system.