

Experiment 3.1: The Ising Ferromagnet

Introduction

If very many particles interact with one another, qualitatively new properties can be the result. For example at low temperatures or high pressures gases suddenly liquify, liquids turn to solids, etc. There are a large number of systems like these which, in thermal equilibrium, change their properties at a well defined temperature. In mathematical modeling such *phase transitions* occur only in infinitely large systems.

Is it possible to simulate thermal equilibrium and slowly heat up or cool down a system on a computer? Can the simulation of finite systems describe phase transitions? In this experiment you will investigate these questions using as an example the Ising ferromagnet on a square lattice.

Objectives

- To develop code for the numerical simulation of the properties of a 2-D Ising ferromagnet
- To use the model to calculate the magnetisation as a function of temperature
- To investigate the divergence of the correlation length and the critical slowing down close to the transition temperature.

Outline of the model

Description of the properties of a system in thermal equilibrium is based on the calculation of the partition function Z given by

$$Z = \sum_{\underline{S}} \exp(-H(\underline{S})/k_B T). \quad (1)$$

Z is the sum over all possible states of the system \underline{S} and each state is weighted according to its energy $H(\underline{S})$. T is the temperature and k_B is the Boltzmann constant.

The aim is to investigate the Ising model of a ferromagnet. This is the simplest model of a ferromagnetic system. We consider a square lattice occupied by magnetic spins which can only take two possible orientations. There is an interaction between the spins which gives rise to the magnetised state. Mathematically this is formalised as follows: For every lattice site $i = 1, \dots, N$, there is a (spin) variable $S_i \in \{+1, -1\}$ such that the multispin state is identified by $\underline{S} = (S_1, S_2, \dots, S_N)$. The forces which give rise to the ferromagnetic state are very short ranged and can be taken to involve nearest

neighbours only. Consequently the energy of the system consists of a summation over nearest neighbours $(i, j)_{nn}$ as well as over all sites i .

$$H = -J \sum_{(i,j)_{nn}} S_i S_j - h \sum_i S_i. \quad (2)$$

The term proportional to h describes the effect of an external magnetic field which has the effect of aligning the spin parallel to h .

In principle one now has to calculate the partition function using equ 1 in order to evaluate average quantities, since each state \underline{S} has a probability $p(\underline{S})$ given by

$$p(\underline{S}) = Z^{-1} \exp(-H(\underline{S})/k_B T). \quad (3)$$

We can then calculate the thermodynamic average of some quantity $A(\underline{S})$ from

$$\langle A \rangle = \sum_{\underline{S}} p(\underline{S}) A(\underline{S}). \quad (4)$$

In practice this is an extremely inefficient way of calculating averages since Z can only be calculated from eq 1 for very small systems. This is because the probability of a given state is very strongly peaked close to the equilibrium value and if we try to calculate Z via standard numerical integration techniques we spend a lot of time in states which have a rather low probability. A better way to calculate thermodynamic averages is to use the technique of *importance sampling*. To this end a transition probability $W(\underline{S} \rightarrow \underline{S}')$ between two states \underline{S} and \underline{S}' is defined such that the following *detailed balance condition* is obeyed

$$W(\underline{S} \rightarrow \underline{S}') \exp(-H(\underline{S})/k_B T) = W(\underline{S}' \rightarrow \underline{S}) \exp(-H(\underline{S}')/k_B T). \quad (5)$$

The physics of this can be understood given that the probability of occupation of a given state $p(\underline{S}) = Z^{-1} \exp(-H(\underline{S})/k_B T)$. This means that in thermal equilibrium \underline{S} is a stationary state, by which we mean that $p(\underline{S})$ does not change with time. We have to make sure that W is able to cover the whole configuration space defined by the set of states \underline{S} . Here we will use the Metropolis algorithm, probably the most common form.

The stochastic process defined by W leads to a sequence of physically relevant states, $\underline{S}(0), \underline{S}(1), \dots, \underline{S}(t)$. Within these states averages can be calculated as follows:

$$\langle A \rangle_{t_0, t_1} = \frac{1}{t_1 - t_0} \sum_{t=t_0}^{t_1} A(\underline{S}(t)). \quad (6)$$

in the limit $t_0 \rightarrow \infty$ and $t_1 \rightarrow \infty$ the average agrees with the statistical average (eq 4). What this means is that we have to allow the simulation to proceed for some time to reach equilibrium and then average for a further time period to obtain the average. Note that these averages are described as time averages. However, the Monte-Carlo method does not give us a specific timescale, since we are just taking steps through phase space, which in general have an unknown associated timescale. However, it is often useful to think of the Monte-Carlo moves as representing a dynamic evolution of the system state, with time represented in 'Monte-Carlo moves per particle'. Thus in eq 6, t_0, t_1 are integer timesteps, measured in Monte-Carlo moves.

Boundary conditions

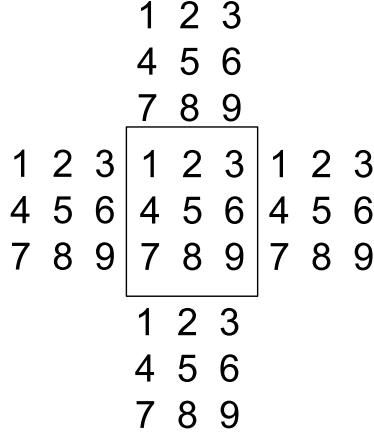


Figure 1: Illustration of Periodic boundary conditions for a 3×3 system.

Theoretically the phase transition occurs only for an infinite system, which is of course not realisable in a numerical simulation. In order to reduce the effects of the finite size we use *Periodic Boundary Conditions*. What this means is that we create replicas of the computational cell translated in space by the size of the cell; effectively a spin on one boundary is assumed to be a neighbour of the spin on the opposite boundary. This is illustrated in fig 1, which shows periodic boundary conditions applied to a 3×3 array. The computational cell (surrounded by the solid line) is translated in 2-D, the effect of which, for example, is that spins (1,4,7) become neighbours of spins (3,6,9) *and therefore interaction between these spins must be allowed when calculating the energy*. The algorithm for this will be described later.

The Metropolis algorithm

The Metropolis algorithm involves making a change in the configuration of the system, $\underline{S} \rightarrow \underline{S}'$ and allowing the change with a probability of unity if $H(\underline{S}') < H(\underline{S})$, that is all moves decreasing the energy are allowed. Otherwise the change is allowed with a probability $p = \exp(-(H(\underline{S}') - H(\underline{S}))/k_B T)$. It can be shown theoretically that such changes satisfy the detailed balance condition. The algorithm to do this is as follows:

1. For a given state choose a spin i (randomly or sequentially), change the direction of the spin, and calculate the energy change ΔE .
2. If $\Delta E < 0$, allow the spin to remain in the new state. If $\Delta E > 0$, choose a uniformly distributed random number $r \in [0, 1]$. if $r < \exp(-\Delta E)/(k_B T)$ allow the spin to remain in the new state, otherwise the spin reverts to its original state.
3. Iterate steps 1-2.

Calculation of the energy change

The energy difference is easy to calculate since we can write the energy of state \underline{S} as

$$H(\underline{S}) = -2JS_i \sum_{j \in \mathcal{N}(i)} S_j - hS_i + \text{remainder}, \quad (7)$$

where $\mathcal{N}(i)$ is the set of nearest neighbours of spin i , that is the sum in eq 7 is *over nearest neighbours only*. The 'remainder' term contains the contribution of all other spins, which of course does not depend on S_i . If we now flip the direction of the spin, ie $S'_i = -S_i$, the energy has the same remainder term as in eq 7, so it is straightforward to show that the energy change is

$$\Delta E = -2S_i \left(J \sum_{j \in \mathcal{N}(i)} S_j - h \right) = -2S_i h_i, \quad (8)$$

where h_i is the *internal field* acting on spin i ,

$$h_i = J \sum_{j \in \mathcal{N}(i)} S_j - h \quad (9)$$

Pre-calculation of the probabilities - a 'trick of the trade'

For every spin at each point in the Monte-Carlo simulation we need to calculate the probability of a change of spin state. In principle, this can be done by evaluating the internal field from eq 9, followed by the energy change from eq 8 and finally the probability of reversal $\exp(-\Delta E/(k_B T))$. This requires significant CPU time, especially the calculation of the exponential. However, this process can be speeded up considerably in the case of Ising spins, which have only two allowed states $(+1, -1)$. With 4 nearest neighbouring spins having 2 possible states there are only 2^4 spin configurations and hence a total of 16 internal fields (some of which are degenerate). Given that the starting state of spin i can be $(+1, -1)$ there are a total of 32 probabilities for reversal of the spin. This makes it feasible to pre-calculate the probabilities at a given temperature and simply look up the probability from the precalculated array. For a spin at a lattice point (i, j) the probability is calculated from an array having the following sort of structure.

$$\text{probability}(S(j-1, i), S(j+1, i), S(j, i-1), S(j, i+1), S(i, j)).$$

Here, $(S(j-1, i), S(j+1, i), S(j, i-1), S(j, i+1))$ are the nearest neighbour spins of the lattice point (i, j) , and $S(i, j)$ is the spin at (i, j) . In the code we simply have to calculate the reversal probability and then allow the change if the random number $r < \text{probability}(S(j-1, i), S(j+1, i), S(j, i-1), S(j, i+1), S(i, j))$. Clearly other data structures are possible, the choice is yours. The 'trick' is to create an algorithm to populate the probability array with all the possible spin configurations and the resultant probabilities.

Experiment

The experiment is based principally on the calculation of the relevant order parameter for the transition, in this case the magnetisation, defined as

$$M(T) = N^{-1} \sum_{i=1}^N S_i, \quad (10)$$

where N is the total number of spins. Clearly $M(T)$ can be positive or negative. Below a critical temperature, referred to as the Curie temperature T_c , the system achieves a spontaneous magnetisation - this is the Ferromagnetic state. According to analytical theory $T_c = 2.269J/k_B$.

- First investigate the temperature dependence of the magnetisation $M(T)$ for zero external field. To do this first set the spins in the same direction and then carry out a series of Monte-Carlo moves, each involving a pass through all the spins once, allowing them to change state with the appropriate probability. It is best to average the magnetisation over a few moves following eq 6.

$$\langle M \rangle_{t_0, t_1} = \frac{1}{t_1 - t_0} \sum_{t=t_0}^{t_0+t_1} N^{-1} \sum_i S_i(t). \quad (11)$$

The experiment involves allowing the calculation to run for a large number of moves, averaging over each 10 moves, remembering that t_0, t_1 are measured in Monte-Carlo moves. Over the simulation the magnetisation will evolve to the equilibrium value for the temperature T . Plot $\langle M \rangle_{t_0, t_1}$ as a function of t_0 and determine the equilibrium value $M(T)$ (Save the data for the next analysis). Plot $M(T)$ vs T to determine the Curie temperature - how close is this to the analytical value $T_c = 2.269J/k_B$? Do this for a number of system sizes. Also, take some typical configurations and monitor the change in magnetic state as the transition is approached.

- Critical slowing down. Taking the Monte-Carlo moves as representing a physical time, determine the time taken to reach equilibrium at each temperature. Plot this as a function of temperature. Note the increase as $T \rightarrow T_c$. This is known as 'critical slowing down'. At a phase transition, not only do the fluctuations increase in magnitude, they also become slower.
- The effect of an external magnetic field. Repeat the first part of the experiment with a large external magnetic field. What happens to the phase transition?
- Non-equilibrium states. Start with a system at a high temperature, say $1.5T_c$. Allow enough time to reach equilibrium and then reduce the temperature instantaneously to $0.4T_c$. You should be able to generate states consisting of areas with $S = +1$ and $S = -1$. How do these states vary with time?