Investigation into the Properties of the 2D Ising Model

Emma Hughes

December 2021

1 Introduction

In this report I will create a 2 dimensional Ising model that will be used to represent a ferromagnetic material with the lattice sites representing spins in the material that are able to take on one of two states, up (+1) or down (-1). The effect temperature, grid size and initial conditions have on the Ising model will be investigated. This will done by taking samples of the configuration of the Ising model, using the Metropolis algorithm, at thermal equilibrium under different conditions and comparing results.

2 The Ising Model

The Ising model is a mathematical system consisting of discrete variables, σ_i, that can be in one of two states, +1 or -1. These variables are spread across a square lattice with discrete intervals between the lattice sites. In this report the 2D Ising model will be used to model a ferromagnetic material with the discrete variables at each lattice site representing spin which can be either up (+1) or down (-1). The Hamiltonian of this system can be written as:

$$E(s) = -\sum_{<ij>} J_{ij}\sigma_i\sigma_j - h\sum_i \sigma_i$$

The first summation is taken over interacting spin pairs. Each spin only interacts with the spins directly adjacent to them on the lattice. The second summation is taken over the entire lattice. J_{ij} describes the energy exchange between spin sites, B is the external magnetic field and σ_j represents the individual spins on each of the lattice sites.

If $J_{ij} > 0$, neighbouring spins tend to align, meaning the material is ferromagnetic. If $J_{ij} < 0$, neighbouring spins tend to anti-align and so the material is anti-ferromagnetic. If $J_{ij} = 0$, there is random spin alignment and so the material is non-ferromagnetic. The magnitude of J_{ij} indicates how strongly neighbouring spins are coupled to each other.

In this model we take the external magnetic field to be zero, reducing the Hamiltonian to:

$$E(s) = -\sum_{<ij>} J_{ij}\sigma_i\sigma_j$$

3 Metropolis Algorithm

In order to draw sample configurations of Ising systems at thermal equilibrium, the Metropolis algorithm is used which is described below.

1. We have an NxN lattice of randomly assigned spin states.

2. A spin is flipped and the change in energy of the system, ΔE, caused by this flip is calculated.

3. If $\Delta E < 0$, meaning the system is brought to a state of lower energy, the flip is accepted and the spin site remains in this new state.

4. If $\Delta E > 0$, meaning the system is brought to a state of higher energy, the flip is accepted with probability $(e^{-\frac{\Delta E}{kT}})$ or rejected with probability $(1 - e^{-\frac{\Delta E}{kT}})$. If the flip is rejected, the spin of the system is flipped back so that the system is in its original configuration.

5. The process is repeated.

One Metropolis step is described by points 2-4. In order to use the Metropolis algorithm to obtain sample configurations at thermal equilibrium we must allow a given number of metropolis steps to be carried out and not stored in order to allow the system to reach thermal equilibrium before storing data. After this, a number of metropolis steps are taken, their values recorded and averaged to produce a result.

4 The Effect of Temperature

It is clear to see from the probabilities of flip acceptance or rejection that the temperature of the system has an effect on the resulting configuration of the Ising model, and so we can expect to see significantly different configurations at varying temperatures. To investigate this effect the Metropolis algorithm was used to find the configurations of the Ising systems at thermal equilibrium at various temperatures. This was done multiple times and the results are plotted in Figure 1.

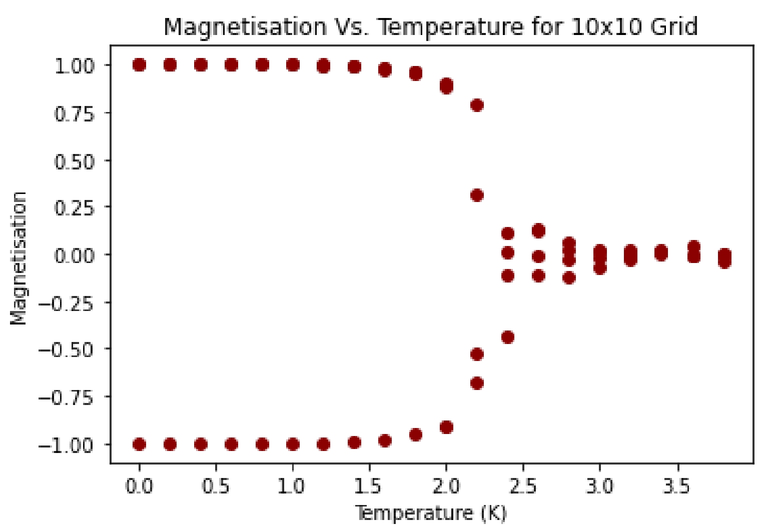

Figure 1: Magnetisation Vs. Temperature

We can see that there is a clear phase transition between 1.5K and 3.0K. At low temperatures (below 1K) the system strongly favours spin alignment (ferromagnetism), that is, either all spins are aligned up (M=1) or all spins are aligned down (M=-1). At higher temperatures ($T > 3.0K$) the system strongly favours random spin alignment (paramagnetism) with no overall magnetisation (M=0).

The Curie temperature (or critical temperature) is defined as the temperature above which certain materials lose their permanent magnetic properties (M=0). For this simulation the Curie temperature is (3.0 ± 0.3)K.

Below the critical temperature, the initial state of the system affects the orientation of the magnetisation of the ferromagnetic material when thermal equilibrium is reached. There is an approximately even split between the number random initial states that result in a magnetisation of 1 and the number that result in a magnetisation of -1. The configuration of the random initial state has no impact on the Curie temperature of the system or the magnetisation at temperatures higher than the Curie temperature.

5 The Effect of Grid Size

We can see that larger grid sizes require more steps to bring the system to equilibrium than smaller grid sizes. In Figure 2 the number of steps required to bring the 2D Ising models of different grid sizes to equilibrium at temperature T = 2.0K are found. We know from Figure 1 that the magnetisation of the Ising model at T = 2.0K when it has reached thermal equilibrium is approximately 0.9.

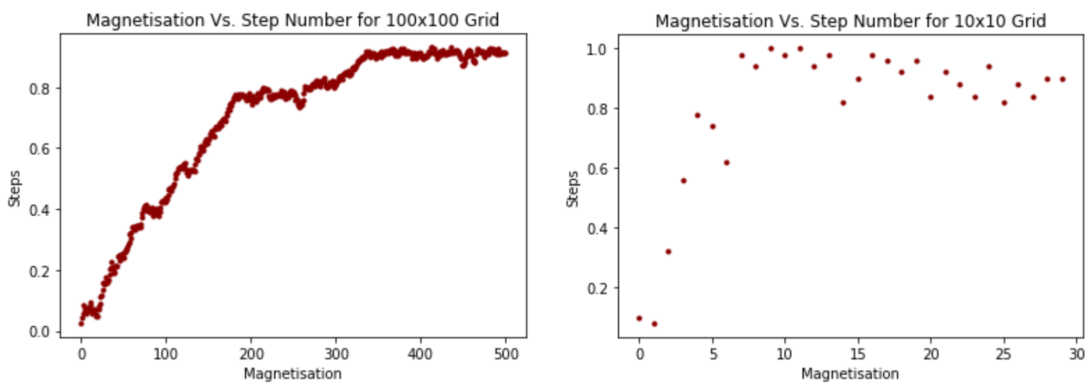

Figure 2: Number of steps required to reach thermal equilibrium for different sized grids.

We can see that 100x100 grid takes about 350 steps to reach equilibrium whilst the 10x10 grid only takes about 10 steps. This that simulations using a 10x10 Ising model can have a much faster computational time as the number of equilibrium steps required to reach thermal equilibrium is much smaller.

6 Bibliography

[1] P. Fendley, Modern Statistical Mechanics. (Currently unfinished as of December 2021).
[2] Huang, K., 2014. Introduction to statistical physics, Hoboken: Taylor and Francis.