Metropolis Algorithm for the Ising Model

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1 Introduction

Magnetism, a fundamental property of materials, arises from the collective behavior of atomic magnetic moments. In ferromagnetic materials, these magnetic moments, or spins, tend to align parallel to each other, resulting in a macroscopic magnetization. The Ising model, proposed by Ernst Ising in 1925, is a simplified representation of this phenomenon. It consists of discrete variables called spins, which can be in one of two states: up (+1) or down (-1). These spins are arranged on a lattice, typically in one, two, or three dimensions, and interact with their nearest neighbors.

The Hamiltonian of the Ising model, representing the energy of a given configuration of spins, is given by:

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j - B \sum_i \sigma_i \tag{1}$$

- J : Coupling Constant. If J ¿ 0, the material is ferromagnetic, neighbouring spins will tend to allign. If J ¡ 0, the material is anti-ferromagnetic.
- ¡i,j¿ : This represents a summation over all interacting spins. In this case we only consider adjacent atoms.
- B : This represents an external magnetic field.

Ferromagnetism sometimes occurs in materials below their Curie Temperature T_C. Microscopic domains within the material will experience magnetic moment allignment, however macroscopically over the whole material the orientation of these microscopic domains is random, hence the material exhibits no net magnetism. If a magentic force B is applied to the material, these domains become alligned and a net magnetisation is observed (this is known as remanensce). Above the Curie Temperature thermal motion is enough to disrupt this magnetization however.

Our project implements a simplified version of the Ising model, where we only consider a 2D square lattice. We also impose periodic boundary conditions,

where edge atoms interact with the opposing edge atoms. This project will attempt to determine if the Crystal Lattice has undergone a Phase Transition from Ferromagnetism to Paramagnetism. This occurs at the Curie Temperature T_C for the lattice.

1.1 Observables

Several variables will be tracked in this simulation, with particular attention paid to how they depend on temperature. Firstly, we'll look at the average Energy per spin, which can be calculated by the following:

$$\langle E \rangle = \left\langle \sum_{<i,j>} H_{i,j} \right\rangle = \frac{1}{2} \left\langle \sum_{i,j} H_{i,j} \right\rangle \tag{2}$$

The half here just accounts for the fact that by summing over every element, we'll count each interaction twice. By plotting $\langle E \rangle$ against temperature, we should see continuous values, with a point of inflection at the phase transition, where the system becomes paramagnetic, and the magnetic moments become random and disordered.

The average magnetization per spin can also be calculated by:

$$\langle M \rangle = \frac{1}{N^2} \sum_i \sigma_i \tag{3}$$

By plotting this value against an iteration count using the Metropolis algorithm, it can be seen if the state approaches a continuous value or not, indicating equilibrium. This continuous value can then be used to determine whether the system acts as Ferromagnetic at that temperature or not. A value of $\in$ [-1,1] indicates Ferromagnetism, as it indicates the magnetic moments have aligned macroscopically across the lattice, whereas a value of 0 indicates paramagnetism, as the spins have becomes unaligned and disordered. This value can also be used to determine the T_C of the lattice. If $\langle |m| \rangle$ (after equilibrium) is plotted against a series of T values, the point of inflection in the graph should be sufficient to determine the T_C value.

The Specific Heat Capacity C_V can be derived, and subsequently calculated as seen below:

$$C_V = \frac{\partial \langle E \rangle}{\partial T} \tag{4}$$

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

HEre Z is the Partition Function, k_B is the Boltzmann Constant, and $\beta = \frac{1}{k_B T}$. In the final step in (5) we used a known result for the derivitce of $\langle E \rangle$ with respect to β rather than explicitly deriving it.

Similarly, the Magnetic Susceptibility χ can be expressed as:

$$\chi = \frac{\partial \langle M \rangle}{\partial \beta} = \beta \left(\langle M^2 \rangle - \langle M \rangle^2 \right) \tag{6}$$

2 Metropolis Algorithm

The Ising model consists of a grid (usually 2D) of spins, where each spin can be in one of two states: +1 (up) or -1 (down). The goal is to understand the behavior of these spins at different temperatures, particularly their tendency to align with their neighbors, which results in ferromagnetism.

2.1 Steps involved in the Metropolis Algorithm for the Ising Model

2.1.1 Initialization

- Create a 2D Lattice of spins, of side length L, where each site in the lattice can have a spin of (+1) or (-1).
- Set a Temperature T for the problem.

2.1.2 Iteration

- **Select a Spin**

  Randomly select a spin σ_i from the lattice.

- **Compute Energy Change**

  Calculate the change in energy ΔE if the spin σ_i were to be flipped. The energy of a spin configuration in the Ising model is given by (1) of this document. If this change is negtive accept the change.

  If it is positive, generate a random number r, if this number is less than the probability criterion $e^{\frac{\Delta E}{k_B T}}$, accept the change. Do not if it is greater.

  Repeat the process for a sufficient number of iterations to allow the system to reach equilibrium.

2.1.3 Repeat for Different Temperatures

- To study the temperature dependence, repeat the above steps for various temperatures T.

2.1.4 Output

- Analyze the spin configurations to study properties such as Magnetization $\langle|m|\rangle$, Specific Heat Capacity C_v, Energy $\langle|E|\rangle$ and Magnetic Susceptibility χ_M.

3 Average Magnetization per Spin versus Temperature

In this section we will investigate the effect of Temperature on the Average Magnetization per lattice site. We will see how it effects the amount of time required to reach equilibrium, and also how it affects if the system will even reach equilibrium. As we can see in figure 1, where the Metropolis Algorithm

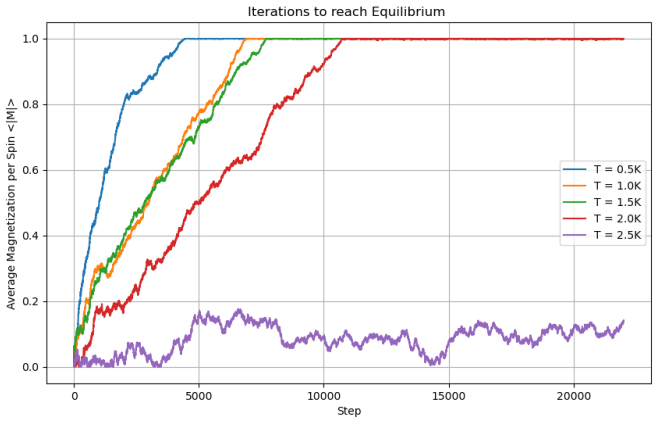


Figure 1: Average Magnetizations per Lattice Site for a (50x50) 2D Lattice for a series of Temperature values

was implemented for various temperatures on a 2D lattice, increasing the Temperature from 0.5K to 2K increased the amount of time (iterations) it took to reach equilibrium. Note that the absolute value of spin was used in this case, as spins of ± 1 are equivalent.

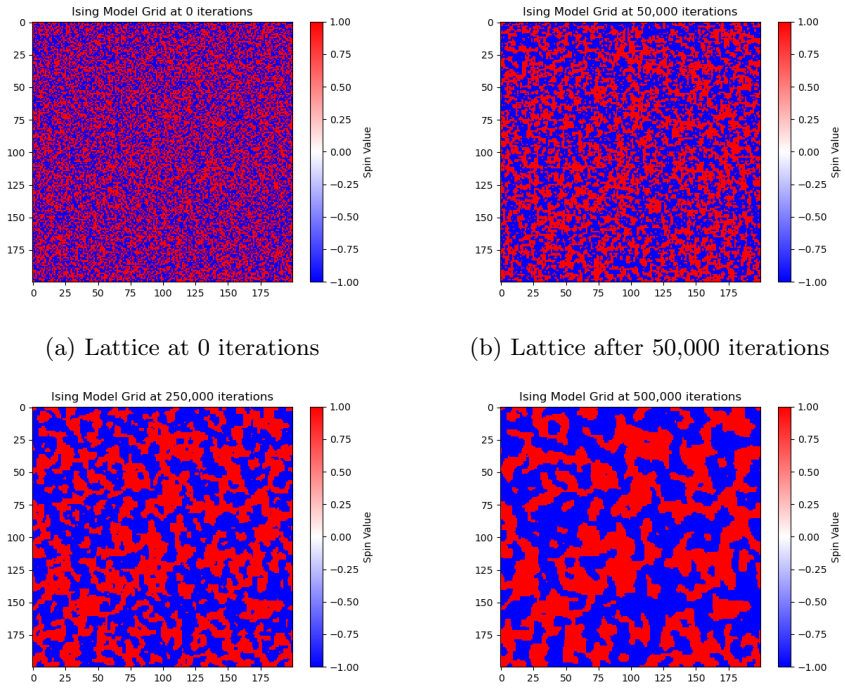
If we look at the Hamiltonian in (1) involved in the ΔE calculation it has no temperature dependance. However, if we look at the probability criterion discussed in section 2.1.2, it is determined by choosing a random number $r \in$ [0,1] and checking if it less than the value $e^{\frac{\Delta E}{K_B T}}$. If T is increased in the denominator here, it decreases the exponent as a whole, making the entire term smaller. Therefore less random numbers will be less than this threshold value, which explains why the system would take longer to reach equilibrium state.

Also interesting to note from figure (1), that a T of 2.5K does not reach equilibrium. This indicates that this value is above the Curie Temperature, therefore the system is paramagnetic. This means that no microscopic domains of aligned spins form within the magnetic, and the magnet as a whole will not act as a ferromagnet. Therefore, we now know that the Curie Temperature is between 2 and 2.5. Drum roll, it is. The Curie Temperature for a 2D Lattice is given by:

$$K_B T_C = \frac{2J}{ln(1+\sqrt{2})} \approx 2.27K \tag{7}$$

In section 4 of this project, we'll investigate this value a bit more.

Also, out of interest. The domains alluded to in various sections of this project. What do they look like I hear you think? Let's take a look. For a sample lattice of dimensions (300x300), see the below plot for a visualisation over iterations of what occurs during the Metropolis Algorithm: We can see above in figure 2, the



(a) Lattice at 0 iterations

(b) Lattice after 50,000 iterations

(c) Lattice after 250,000 iterations

(d) Lattice after 500,000 iterations

Figure 2: Evolution of Magnetic Domains in our Crystalline Lattice as the Metropolis algorithm progresses

microscopic magnetic domains in which the spins are aligned evolve from (a) to

(d). These regions contribute to the macroscopic magnetic moment of the lattice as a whole. The above simulation was for a 200x200 lattice at a temperature of 0.5K which is below the Curie Temperature discussed previously. Therefore we know that this lattice will exhibit ferromagnetic behaviour (i.e. all spins will align) as the algorithm progresses. This means that either the (+1) domains will consume the lattice, or the (-1) will after a certain number of iterations.

4 Observables

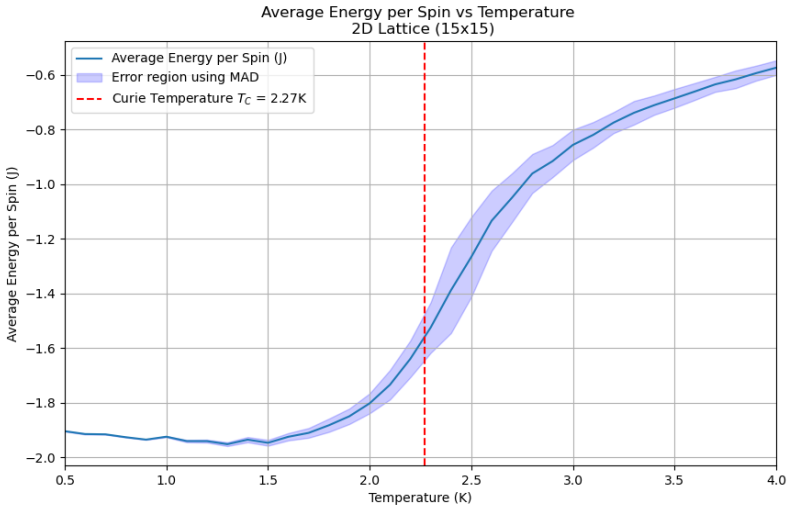
As part of this simulation of a ferromagnet, we are able to use the Monte Carlo aspect of the Metropolis algorithm to calculate the Specific Heat Capacity C_V & Magnetic Susceptibility χ_M of our lattice as a function of temperature.

If we set T = 0.5K, and increment in 0.1K steps beyond the Curie Temperature we will see a Phase transition from Ferromagnetism to Paramagnetism in our system. If we simulate the Metropolis Algorithm at each T value, and allow they system to reach equilibrium (if it even will at the T in question) then we can track the aforementioned observables as well as the Energy & Magnetization per spin to show this Phase Transition has actually occurred. In the below section, at each temperature we allowed the Metropolis Algorithm to run for 75,000 iterations for a (15x15) lattice. Note also, due to statistical noise in these measurements, we iterated the implementation of the Metropolis Algorithm from 0.5K to 4K 200 times in an attempt to reduce the noise, which is still present in these results. Therefore, each point in these graphs is the average of 200 simulations of the exact same simulation. The error bars were calculated using the Median Absolute Deviation (MAD) value of the 200 measurements. This measure is less sensitive to outliers than Standard Deviation. These values were calculated using the Robust Module from the StatsModel Library in Python, using Jupyter Notebooks.

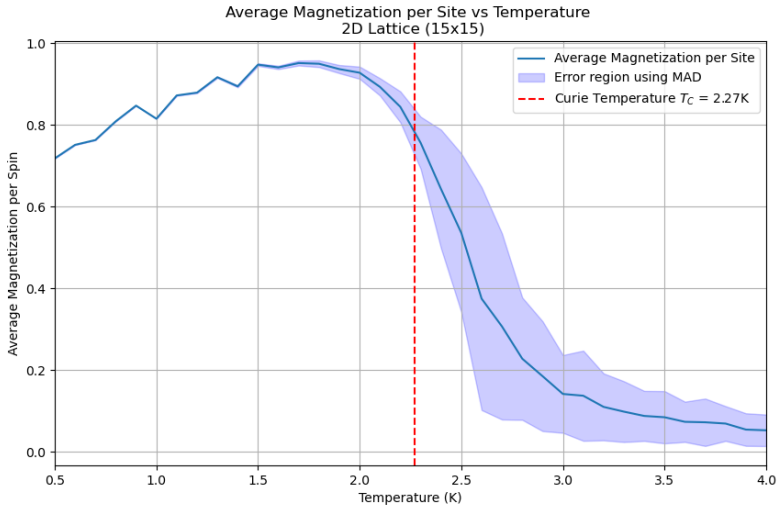
4.1 Average Magnetization & Energy per Spin

We will first initially look at the Magnetization & Energy per Spin. For these observables in the C++ code, we stored the average energy & per spin at each iteration in a vector of doubles. We then only used the average value of the last 25,000 vector elements at each temperature, as it was known from previous simulations that the system had *most likely* reached equilibrium by that point.

Looking at figure 3(a), we can see that $< |E| >$ is roughly at -2J for $\in$ [0.5K, 1.8K]. This agrees with the theoretical prediction for a ferromagnet, where the maximum energy of an alligned system is given by -2J. Intuitevely, this makes sense. Each site, in a perfect allignment, has a spin $\sigma_{i,j}$ of -4 (where B = 0, K_B = 1, and J the coupling constant is 1). However, total energy is divided by 2 to avoid double counting spins, therefore we get -2. Also, this graph shows the increase in energy with temperature increase.



(a) Average Energy per Lattice Site versus Temperature values



(b) Average Magnetization per Lattice Site versus Temperature values

Figure 3: Average Magnetization & Energy per Spin for a (15x15) 2D Lattice

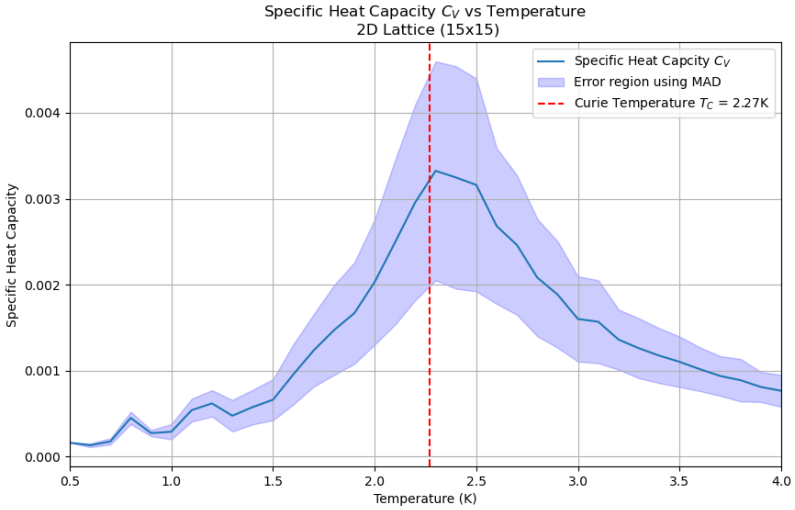
Figure 3(b) shows the Average Magnetization per spin versus Temperature for our lattice. The sharp decrease in magnetization at $T_C \pm 0.2K$ can be seen. This indicates a transition from an ordered state to an unordered state, with opposing spins cancelling each other out and therefore reducing overall average spin. The graph trailing off to 0 indicates this is the long term behaviour, indicative of paramagnetism. See for T = 2.5K, this expains the behaviour seen in figure 1 for that temperature. However, we do have some problematic behaviour in the interval $\in$ [0.5, 2.27]. These values should be approaching , if not equal to 1. This indicates to me that the system is only *approaching* equilibrium after $\approx$ 75,000 iterations at these temperatures, and has not fully become uniform. We may have a situation similar to figure 2 (d) on our hands. If the algorithm was allowed to run for longer at each value this may have been a non-issue. However due to computational and time limitations we did not repeat the simulation with more iterations.

4.2 Specific Heat Capacity and Magnetic Susceptibility

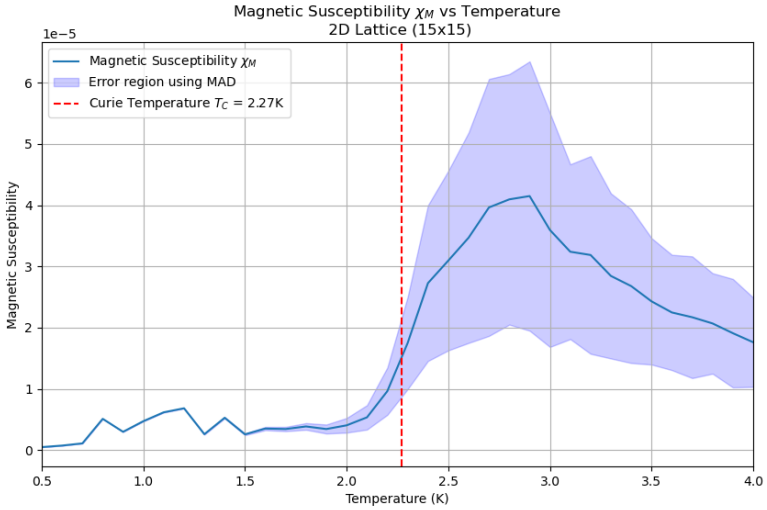
Calculating these observables really showed the usefulness of Monte Carlo simulations. These measures were calculated almost identically, using formulas (5) and (6), which had a nearly identical prefix, and just used the variance in Energy and Magnetization respectively.

In figure 4(a), we can see (what should be) a peak at T_C. From the literature it is known that this peak indicates a phase transition from an ordered state at lower temperatures to disordered state at higher temperatures. This peak in C_V is indicative of the system using an increased amount of energy in reconfiguring the spins to different orientations to achieve this disordered state. We also see a large amount of error at this apex, with slightly smaller error either side. Also, this peak indicates that the phase transition is second order.

Similar for 4(b) for χ_M we see a sharp increase at the Curie Temperature. We also see a large amount of uncertainty in measurements post T_C, perhaps a consequence of this increased disorder.



(a) C_V(T)



(b) χ_M(T)

Figure 4: Specific Heat Capacity and Magnetic Susceptiptibility versus Temperature for our (15x15) 2D Lattice