Using the Ising model to study aspects of Ferromagnetic systems

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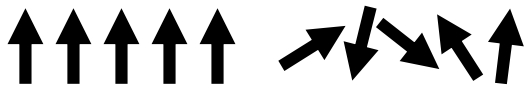
Abstract

Using a Metropolis Monte Carlo Simulation of the Ising model, the spin microstates of ferromagnetic systems were studied. The speed at which the system reaches thermal equilibrium increased the closer its temperature got it Curie Temperature. At thermal equilibrium, the system's energy increased with temperature. The system's magnetisation was either ±1 at low temperatures or 0 at high temperatures, with a dramatic phase transition when its temperature increased to its Curie temperature. The Mean Field theory gave an accurate approximation for the Ising model's magnetisation at low temperatures. But did not exhibit the systems dramatic phase transition as the temperature approached the Curie temperature, instead gradually transitions over a large temperature range. The magnetic susceptibility of the Ising Model remained independent of temperature, until it approached the system's Curie temperature, where the susceptibility increased with temperature.

Introduction

Inside Ferromagnets, their spin magnetic moments algin themselves in the same direction [1]. This is due to the strong interaction between the magnetic moments, creating a lower energy state for aligned ordering than random. Ferromagnetism is only exhibited in low temperatures, up to the Curie temperature, T_c [2]. For temperatures above T_c, ferromagnets loss their aligned ordering as the spin magnetic moments rotates in random directions, transitioning into a paramagnetic state



Ferromagnetism **Paramagnetism**

Figure 1. Arrangement of spin states while experiencing ferromagnetism (left) and paramagnetism (right)

Ising Model

To simulate the arrangement of spins in a ferromagnet, and how they change due to temperature, one can use the Ising model [3]. The system is comprised of N number of sites in a square grid, each one either in the up or down spin state, $s = \pm 1$. The energy of a site depends on its own spin and the spin of its nearest neighbours, it can be calculated with

$$\frac{E_i}{J} = -\sum_k s_k s_i, \qquad (1)$$

where E_i is the energy of the spin, s_i is the spin state of the chosen site, s_k are the spin states of the site's nearest neighbours, and J represents the strength of the interaction forces between the sites in units of energy [3]. The adjacent spins create a local magnetic field which influences the direction a spin will align, a spin aligned parallel with its neighbours will have a lower energy than if it were antiparallel. The total energy of the system, E, is just the sum of equation (1) over all N sites, while the system's magnetisation, M,can be calculated with

$$M = \frac{1}{N}\sum_i s_i, \qquad (2)$$

[4]. When the system is subjected to heat, the energy it receives can allow a site to switch spin state, even raising it to a higher energy level. This can be determined by the Boltzmann distribution

$$p_i = exp(\frac{-\Delta E_i}{k_B T}). \qquad (3)$$

where p_i is the probability of a site switching its spin state, k_B is the Boltzmann constant, T is the temperature of the system, and ΔE_i is the difference between the energy of the site's initial spin state to the other spin state[5]. If ΔE_i is negative, it will much more likely switch than if it were positive, showing the preference for the state with a lower energy. However, the probability to change to a higher energy state is not zero, with it increasing as temperature increases.

The arrangement of all the spin states in the system will create a microstate, when a site switches spin state, it changes to a different microstate. Over a long period of time, where most of the sites have had the chance to change their spin state, the system reaches thermal equilibrium [2]. This is where the rate at which the system switches from one microstate to another, equals the rate at which the system switches back to the original microstate. Meaning the system's total energy and magnetisation converge to a constant value.

Metropolis Monte Carlo Simulation

To implement the Ising model computationally, a C++ script was created. A 40x40 square grid was created, as shown in figure 2. Each point had a cartesian coordinate, relative to the first site, and either an up (blue) or down (green) spin state. The system had an

inverse temperature variable, β, which could be called up or changed with a function. It had dimensionless units and was calculated by

$$\beta = \frac{1}{T_0} = \frac{J}{k_B T}, \qquad (4)$$

where T_0 is the dimensionless temperature, and T is the temperature in kelvin. Metropolis Monte Carlo was used to simulate whether a site switches spin states due to heat energy in the system [6]. A site is picked using a random number generator, then ΔE_i was calculated for it. If $\Delta E_i > 0$, a random fraction was generated and compared to p_i of the site. If the fraction was less than or equal to p_i, the site switched spin states, while if the fraction was larger, the sites did not switch. If $\Delta E_i < 0$, it was assumed $p_i = 1$ and the site always switched spin state. This was repeated over many iterations to bring the system into thermal equilibrium.
Once equilibrium was reached, the E/J and M can be calculated, with equations (1) and (2) respectively, for the whole grid. To calculate the nearest neighbour spins for the sites at the edge of the grid, the corresponding site on the other side of the grid were used, acting as if the grid had periodic boundaries.

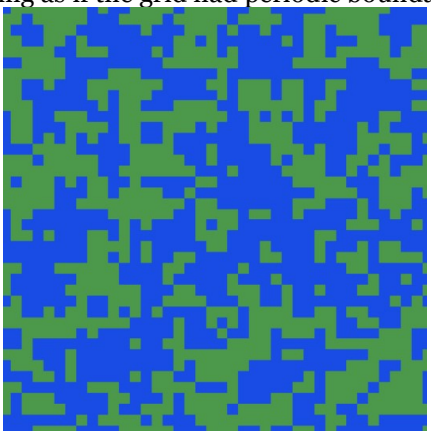


Figure 2. An iteration of the simulated Ising model during thermal equilibrium, at $\beta = 0.25$.

Convergence to Equilibrium

To show that the system converges to a thermal equilibrium, M and dimensionless energy per spin site, E/JN, were calculated using equations (2) and (1), at each iteration up to 500. This process was repeated 50 times, then the average of M and E/JN at each iteration were calculated, as to give an expected value at each iteration. This was repeated for different β and plotted on the same graph in figure 3.

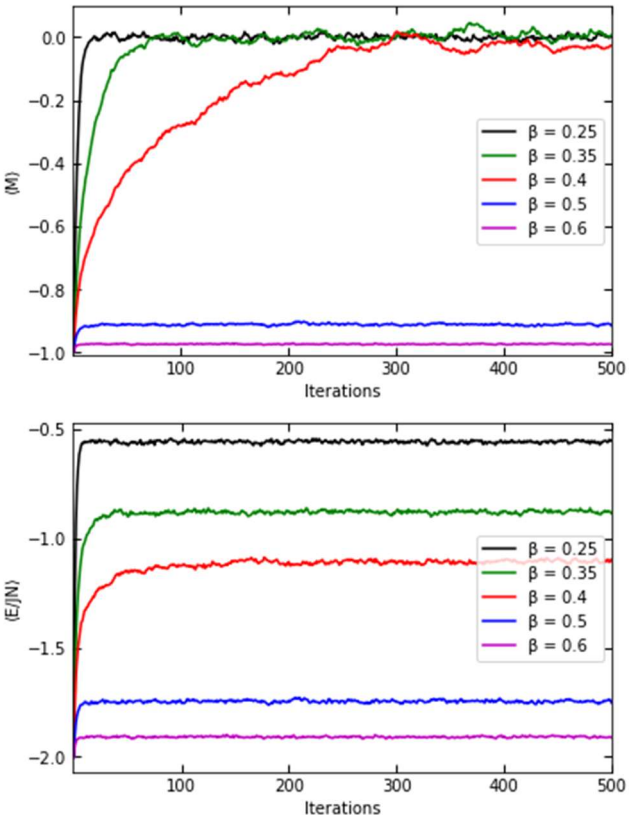


Figure 3. Average M (top) and average E/JN (bottom) against iterations of the Ising model simulation. Each line represents the different β the simulation was running at: 0.25 (black), 0.35 (green), 0.4 (red), 0.5 (blue), and 0.6 (purple).

$\langle M \rangle$ for all the temperatures converge to a constant value, as seen in figure 3. For high β, therefore low system temperature, $\langle M \rangle$ stays close to its oringla value, converging close to -1. This shows the ferromagnetism state continues during thermal equilibrium, as the spin states stay mostly aligned in the same direction. For low β systems, $\langle M \rangle$ converges to 0, as they fluctuate around the value. This shows the systems transition to a paramagnetic state at thermal equilibrium, as a this indicates there is not a favoured spin direction, it is equally likely to be in the up or down spin state. So, the neighbouring spin states of a given site have no effect on the site's spin.
In terms of speed of convergence, both very high and low β systems reach equilibrium quickly, within the first 100 iterations. However, systems with their temperature near T_c will take much longer, the system with $\beta = 0.4$ in figure 3 took more than 10 times as many iterations to reach a constant value than the other systems tested. This suggests that as a system approaches its T_c, and transitions from one state to the other, the speed at which thermal equilibrium is reached increases.
$\langle E/JN \rangle$ also converged to a constant value for all system temperatures. However, unlike $\langle M \rangle$, the converging value is depenatnt on the system's temperature. As β

increases, so the temperature decreases, $\langle E/JN \rangle$ gets more negative.
This indicates that the systems that are in a paramagnetic state, are at a higher energy microstate than the systems exhibiting ferromagnetism. This higher energy allows for the sites to misalign their spin compared to their neighbours. This is consistent with equation (3), the higher energy result in a higher spin state switching probably.

Equilibrium values

Once the systems reach thermal Equilibrium, their properties can be measured to see more clearly how temperature affects it. After 1000 iterations, the average E/JN, and modulus of M ($|M|$) were calculated for the whole system over 50 iterations. This was repeated for different T_0 and plotted on the same graph, in figure 4.

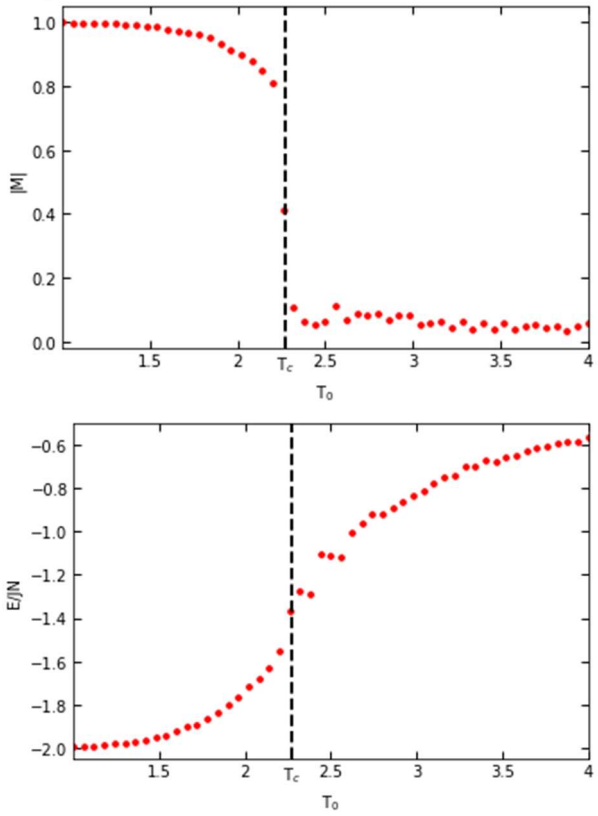


Figure 4. Average$|M|$ (top) and average E/JN (bottom) against T_0. The vertical black dotted line indicates T_c on each graph.

When the system is at low temperatures, $|M|$ remains at a constant of value -1, showing the system is still in the ferromagnetic state as all the spin states are aligned in the same direction. As T_0 increases, $|M|$ slowly decreases as more spin sites switch state due to an increase in p_i.
When $T_0 \approx 2.27$, $|M|$ dramatically decreases to a value just above 0, with it fluctuating about this value as temperatures increases beyond this point. This clearly shows the behaviour of a paramagnet, the spin sites are randomly aligned, with the probability of a site being in a particular state at 50%. This indicates the system underwent a phase transition from the ferromagnetic to the paramagnetic state, with $T_c \approx 2.27 J k_B{}^{-1}$.

In figure 4, E/JN increases gradually for low temperatures. This rate of change increases as the temperature approaches T_c, reaching a maximum gradient at T_c. This suggests that the closer to T_c the system's temperature is, the more the sensitive and susceptible the system is to energy increase. This is explained by equation (3). The percentage of particles that have the minimum energy in the system to switch spin states is based on the Boltzmann distribution [5]. When the temperature reaches T_c, if a site chosen by Metropolis Monte Carlo is in a lower energy spin state, there is a greater chance to switch to the higher energy spin state than stay at the lower energy. This causes the drastic decrease $|M|$ at the phase transition, as a site is more likely to have its spin be misaligned with its neighbours. This causes the system to be in a higher energy microstate and experience paramagnetism.

Exact solution

The exact solution for the magnetisation of a 2D Ising model was found as

$$M = \pm \left[1 - \frac{1}{(\sinh(\frac{T_c}{T} \ln(1+\sqrt{2})))^4} \right]^{\frac{1}{8}}, \qquad (5)$$

[7]. However, this is only valid for temperatures below T_c and assumes the grid lattice is very large. $|M|$ calculated by the exact solution was compared with $|M|$ calculated by the Metropolis Monte Carlo simulation in figure 5.

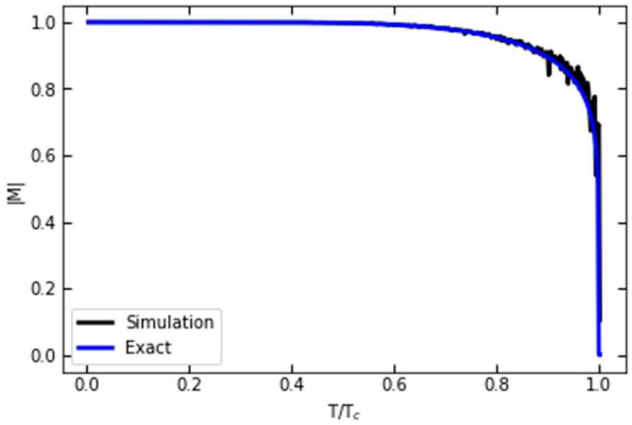


Figure 5. Average $|M|$ against the system's T/T_c calculated with the exact solution from equation (5) (blue), and the Metropolis Monte Carlo simulation (black)

The simulation and exact follow near similar shapes. For low temperatures, the exact solution calculates the same $|M|$ as the Monte Carlo simulation. However, as the temperature approaches T_c, the $|M|$ calculated by

the simulation begins to fluctuate about the $|M|$ produced by the exact solution. The simulation accurately calculates the M at low temperatures, up to $0.8\,T_c$.The main difference between the simulation is that it has a relatively small grid lattice size, only 1600 sites. The exact solution was solved for lattice sizes of orders of magnitudes larger than that, approximating an infinitely large grid. So, as the simulation's lattice size increases, the more it will more precisely fit the exact solution at higher temperatures.

Mean Field Theory

The Mean Field theory can give an approximate solution for the $|M|$ of a ferromagnet at low temperatures, below T_c [8]. It assumes all the sites in the grid lattice display the same behaviour. It averages the local magnetic created by a site's neighbouring particles over every site in the lattice. This effectively places each spin site into its own isolated medium, as seen in figure 6.

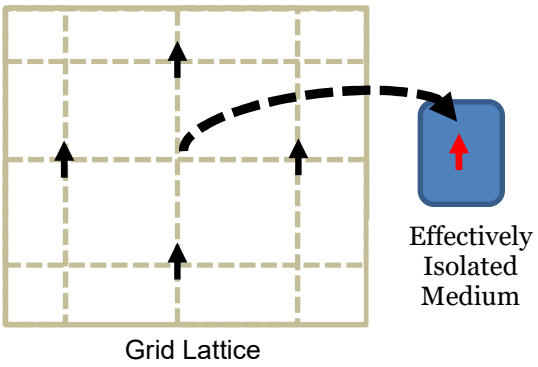


Figure 6. The effective process of the Mean Field Model

The average magnetisation can be acquired by solving this equation

$$|M| = \tanh\left(\frac{4J}{k_B T}|M|\right), \qquad (6)$$

[8]. This shows the benefit of using the Mean Field approximation. A simulation of a whole lattice grid of spin states is not needed to calculate the $|M|$, as all the spin states act identical to each other. The only properties needed is the temperature of the system and J. $|M|$ calculated by the Mean Field theory was compared to the $|M|$ calculated by the Metropolis Monte Carlo simulation in figure 7.

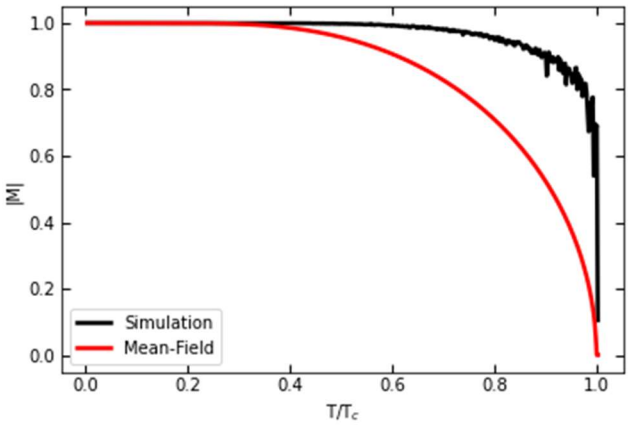


Figure 7. Average$|M|$ against the system's T/T_c calculated with the Mean Field theory (red), the Metropolis Monte Carlo simulation (black),

For low temperatures, the Mean Field accurately approximates $|M|$. It follows the simulation closely, keeping $|M|$ equal to 1. However, the Mean field's $|M|$ begins to decrease at $T = 0.4\,T_c$, at a steady rate. Rather than the dramatic drop that is expected at a higher temperature. This is due to the spin sites in the Mean Field model not interacting with each other.
In the Ising model, if a spin site is the first to switch to a higher energy spin state out of its neighbours, it is more likely to switch back to the lower energy state during the next iteration. This causes the system to keep it's aligned structure at low temperatures, as the sites tend to only stay in a higher energy spin state for a few iterations.
The Mean Field model has an average effective medium that all the sites are in. So, each site is equally likely to switch spin states. As a result, the proportion of sites in the higher spin state is linked to p_i only, not the site's neighbours. As the temperature increase, p_i increases, so does the number of misaligned spin states increases.

Magnetic Susceptibility

The magnetic susceptibility, χ, is a dimensionless quantity the determines the system's M when it is in an external magnetic field, h [4]. For ferromagnetic systems, χ is extremally large compared to other magnetic states. This is due to them already having a M, even when not placed in an external field. It can be calculated by the Ising model by this equation

$$\chi = \frac{\partial}{\partial h}\langle M\rangle = \frac{N}{k_B T} Var(E), \qquad (7)$$

where $Var(E)$ is the variance of the system's energy [9]. The normalized χ was calculated from both the Metropolis Monte Carlo simulation and the Mean Field Theory in figure 8.

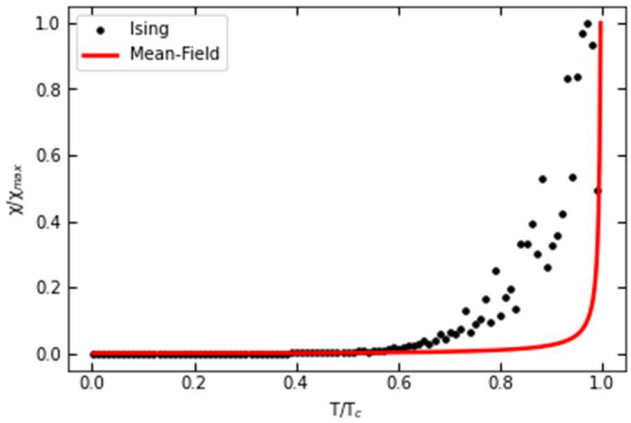


Figure 7. $\chi/\chi_{\max}$ against the system's T/T_ccalculated with the Mean Field theory (red), the Metropolis Monte Carlo simulation (black),

For low temperatures, χ stays at a constant normalised value. This is due to the Ising model's local magnet fields keeping the spins aligned, thus keeping χ at a constant value. But as the system's temperature increases, so does χ.
For the Metropolis Monte Carlo simulation, this increase starts at $0.6T_c$ and steady increases to its maximum at T_c. This Suggesting the system becomes more receptive to external magnetic fields as temperatures increases up to T_c.
This seems to contradict what is expected, as temperature should be inversely proportional to χ due to the increase in energy causes the spin sites to misalign with the external field, reducing M. This suggests that the increase in χ is due to the phase transition at T_c. When the system transitions into a paramagnetic state, the more susceptible to external magnetic fields the system becomes.
This is confirmed by the Mean Field theory, as the increase in χ does not happen until the temperature approaches T_c, suggesting a phase transition for χ. However as seen previously, the Mean Field theory is only accurate for low temperature, so the sharp increase in χ must be ignored.

Conclusion

The Ising model simulation gave insight into ferromagnetic systems and their spin microstate. The system reaches thermal equilibrium after enough iterations, with the number of iterations needed increasing as the temperature approaches the Curie temperature. At thermal equilibrium, the system's energy increased with temperature. The system's magnetisation is either ±1 if in the ferromagnetic state, or 0 if in the paramagnetic state, with a dramatic phase transition when increasing its temperature to its Curie temperature.
The Mean Field theory gave an accurate approximation for the systems magnetisation at low temperatures. But did not exhibit the systems dramatic phase transition as the temperature approached the Curie temperature, instead gradually transitions over a large temperature range.
The magnetic susceptibility of a ferromagnetic system is remains independent of temperature, until the temperature approaches the system's Curie temperature, where the susceptibility increases with temperature.

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