2D Ising Model and AI

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November 2024

1 Introduction

The Ising model is a mathematical model of ferromagnetism in statistical mechanics. It is used to describe the behaviour of magnetic dipole moments, which can be in either the state of spin up or spin down. The spins are arranged in a lattice, and each spin interacts with its neighbours, either aligning with or opposing them. The 2D Ising model is useful for studying critical phenomena, as it undergoes a phase transition at a critical temperature, where it goes from an ordered ferromagnetic state to a disordered paramagnetic state.

The generative AI used to initially model this system is Copilot, an increasingly developing technology that can provide very useful assistance when coding or performing other technical tasks. Integrating AI into scientific simulations, like in this case the 2D Ising model, presents an important intersection of artificial intelligence and physics. The promise of these AI tools lies in their ability to quickly generate functional code, suggest improvements, and facilitate the exploration of complex models with minimal human intervention.

This computational experiment aims to explore the efficiency of AI in simulating the Ising Model and through this, study different variables of this phenomenon.

2 Methods

Copilot was prompted to "generate a Python class to simulate the 2D Ising model on a square lattice using the Metropolis Monte Carlo algorithm". The result was a code that created a class to imitate the model's behaviour and calculated its respective variables. The output given is the final energy and final magnetization. The first change made to the produced code is to add a definition that plots the state of the lattice, using plt.imshow() to display the 2D array of spins as a greyscale image where spin up is black and spin down is white. The second modification made was the inclusion of the 'sweep' parameter in the 'metropolis_step' definition. This is done to include two different ways in which the spins are updated through each iteration. Random spins are chosen for an update for the random sweep. In the sequential sweep, every spin is updated in predictable order. The third improvement is done by defining a new function as '_attempt_flip', which attempts to flip the position of the spin in the lattice. This was previously done in the 'metropolis_step' function but was changed accordingly to make the code more concise and less repetitive. I also removed the 'import random' and modified the code to use the NumPy random function.

The code was then modified to plot the required values. First, we obtain the average magnetization, energy, magnetic susceptibility, and heat capacity as a function of the magnetic field for T = 1.0 and T = 2.0 in a system size L x L = 10. These same quantities are then obtained by setting the magnetic field to zero and finding the critical temperature. Finally, with the obtained temperature, we plot the magnetic susceptibility and the heat capacity as a function of system size.

3 Results

To start, the 2D Ising Model was visualized by using the Metropolis Algorithm in Figure 1. Temperature is set to around T = 2.5, close to the critical temperature, as it allows us to see the behaviour of the Ising model as it undergoes a phase transition. The black and white regions represent clusters of spins in opposite orientations (+1 and -1).

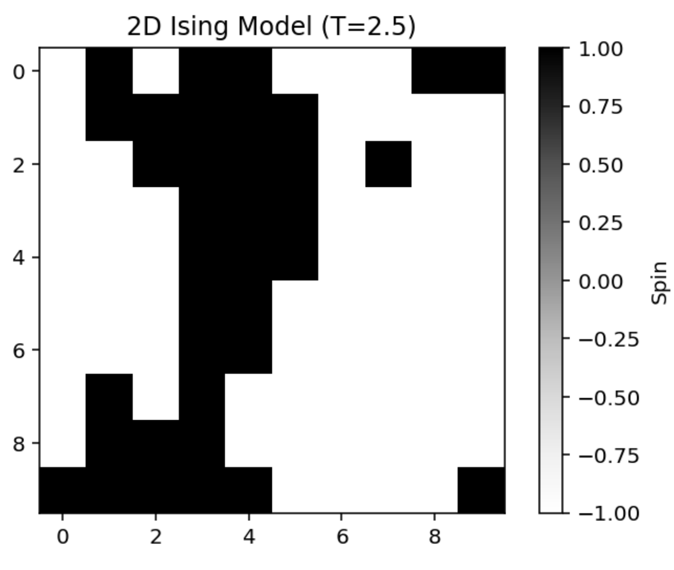

Figure 1: Ising Model, Metropolis Algorithm.

We modify the code to obtain the average magnetization, energy, magnetic susceptibility, and heat capacity as a function of the magnetic field, seen in Figure 2.

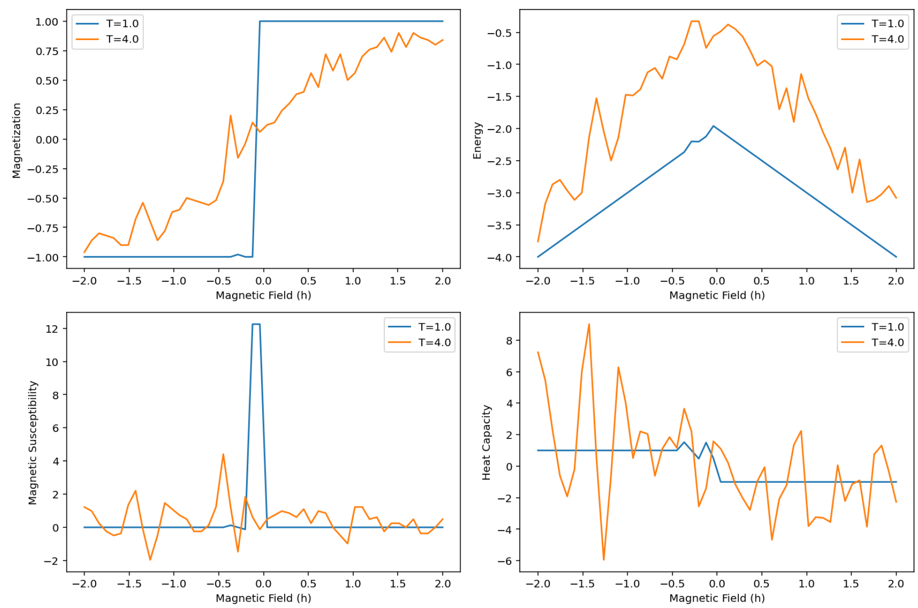

Figure 2: Average magnetization, energy, magnetic susceptibility, and heat capacity as a function of the magnetic field for T = 1.0 and T = 2.0.

The Magnetization vs. Magnetic Field shows the different behaviour of the system when it's under and over the critical temperature value. For T = 1.0, the magnetization jumps suddenly from positive to negative. This is to be expected for the behaviour of the ferromagnetic phase at low temperatures. For T = 4.0, magnetization increases more gradually as the magnetic field increases gradually from negative to positive. This suggests the state is in a paramagnetic phase, where thermal energy dominates, meaning the individual spins in the system are constantly flipping and becoming disordered due to the high temperature. Because the system's natural tendency is to stay disordered, the effect of the field on the spins is weak.

The Energy vs. Magnetic Field plot for both temperatures shows the same overall pattern. For the low temperature, there is a sharp change around h = 0, which reflects the transition in the magnetization. For the higher temperature, the switch is less pronounced, and fluctuations in energy are more pronounced because of the thermal fluctuations that contribute to the system's energy.

The magnetic Susceptibility vs. Magnetic Field plot is a reflection of the Magnetization vs. Magnetic Field. The sharp peak for T = 1.0 occurs at the same point in which the Magnetization switches from negative to positive. For the higher temperature, the change is overall low and has less structure.

The heat capacity measures how much the system's energy changes in response to changes in temperature. Heat Capacity vs. Magnetic Field for T = 1.0 yields a very flat line that is close to zero, which may suggest that variations in the magnetic field do not cause significant energy changes. The line for the second temperature value has higher fluctuations suggesting the higher sensibility to magnetic field changes.

The magnetic field is set to zero to find the critical temperature of the system. The same functions are obtained as a function of the temperature in Figure 3.

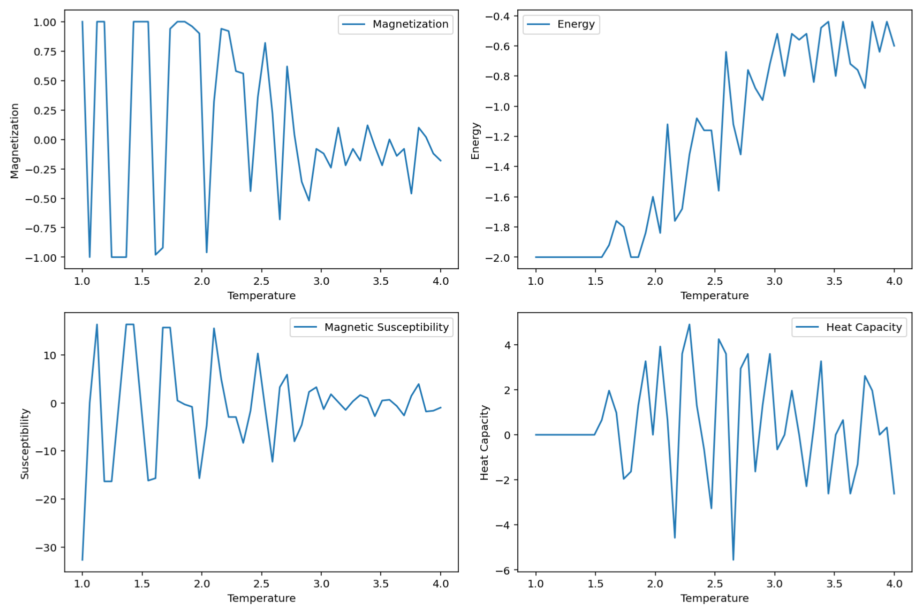

Figure 3: Same quantities as a function of temperature for field=0.

When the magnetic field is set to zero, we can first observe the Magnetization vs. Temperature plot, and how as temperature increases its fluctuations decrease. At low temperatures, the magnetization values vary between positive and negative, as expected. Around T = 2.0 and 3.0, because of the critical value, the magnetization fluctuates rapidly and decreases to smaller values. At higher temperatures, the value fluctuates around zero.

The Energy vs. Temperature plot behaves as expected, with increasing energy as the temperature value increases. Around the critical temperature, the energy increases significantly as thermal fluctuations disrupt the order and cause the spins to become more randomly oriented, leading to higher energy.

The susceptibility, as the magnetization plot, also has decreasing fluctuations as temperature increases. While we can see that it follows the expected trend of decreasing susceptibility as temperature increases, we should not be getting negative values for the plot. This may be due to issues in the calculation method or due to limitations of the simulating model.

The Heat Capacity vs. Temperature graph also shows a similar error, as the negative values are not physically meaningful. We can still observe peaks in heat capacity at the critical temperature, with close to zero values at low temperatures and a tendency to fluctuate and decrease at higher temperatures.

By looking at the peaks in heat capacity and magnetic susceptibility we can see the temperatures at which the system undergoes a phase transition. By finding the maximum value, we can find the temperature at which the system converges between ferromagnetic and paramagnetic phases. The critical temperature is found to be around 2.27°.

Finally, we find the magnetic susceptibility and the heat capacity as a function of system size using the critical temperature. The results are seen in Figure 4. For this code, the number of steps and averages is increased to create a more accurate modelled behaviour.

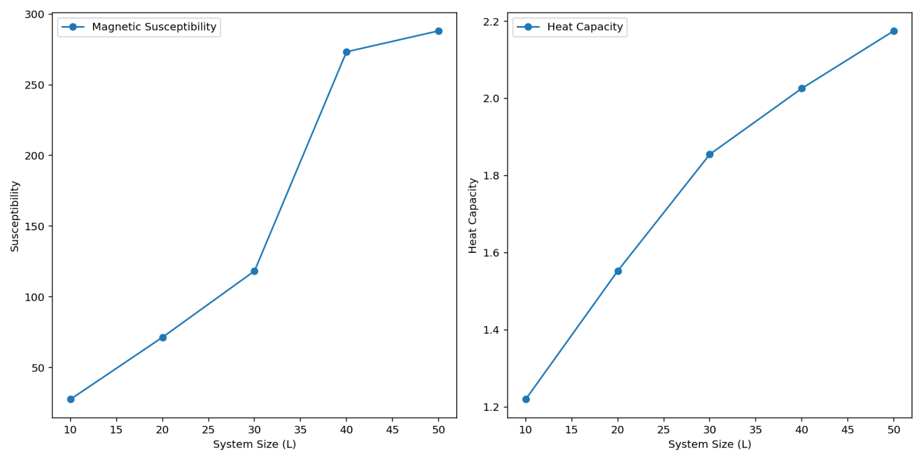

Figure 4: Magnetic susceptibility and the heat capacity as a function of system size for T_c.

Close to critical temperature, we expect the susceptibility to diverge as the system size increases. The increase in magnetic susceptibility indicates that as the system size grows, the spins in the lattice become more correlated and respond collectively to external magnetic influences. The heat capacity plot also shows an increasing trend. Near the critical temperature, the system undergoes large energy fluctuations, which contribute to an increase in heat capacity.

4 Conclusion

The AI as an assistant tool for building computational models was very useful. It created the basis for the necessary code and debug any encountered issues. While it is very useful for constructing the simulating code, it still lacks the necessary human assessment to evaluate the required and reasonable result. The AI-generated code sometimes lacked conciseness, requiring restructuring to make it smoother and easier to debug. For example, functions like metropolis_step and attempt_flip needed human intervention to ensure they were separated to avoid redundancy and improve efficiency. The code also had to be changed to allow for more iterations and increase accuracy, as it could be observed from the results that meaningful errors were made. Nonetheless, generative AI proved to be an extremely useful tool and shows much promise for the future of research and modelling in physics.