Phase Transitions

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1 Introduction

In this project we sought to use a Monte Carlo Markov Chain algorithm to emulate a 2D Ising model, which models a ferromagnet, and experiment with the behavior of the model under different temperatures and magnetic fields.

Specifically, we hope to look at the phase transition that occurs to a material in order to properly estimate the Curie temperature. We also estimate the material reaction to an external magnetic field at various temperatures both above and below the Curie temperature in order to witness the Hysteresis curve.

2 Methodology

2.1 MCMC Method for 2D Ising Model

To begin, we create a grid of specified size and set it to a random state to model the Ising Model. For best results we initialize the state to all positive 1 values. We then calculate the energy of the state by iterating over each grid location and adding together each grid value multiplied by the sum of the four surrounding grid spaces' values. The sum from each grid space is then multiplied by J, a coupling constant, which gives us the energy. The initial sum magnetism of the system is simply the size of our grid as it is equal to each of the ones added together. If we wanted the average magnetism of a state we would just divide the sum magnetism by the size of the grid.

After initializing the system, we then create a new state for the system by flipping the sign of one of the positive 1s to -1. We choose the location of the switch by taking a random integer from 1 to the size of our grid subtracted by 2 in both the x and y directions(this allows us to have ghost cells on the boundary). We then use those values to calculate the random index in which we are flipping the sign of its value. We enforce our periodic boundary conditions here, before we calculate the energy value.

We then can calculate the change in energy from the old state to the new state by summing the neighboring values and multiplying by the random index value. We are also multiplying by two to account for each pair being counted twice. Since we are exclusively working with values of -1 and 1, the sum magnetism can be updated by adding the value of the random index multiplied by two, representing the change in magnetism. The actual magnetism of the state is the sum magnetism divided by the grid size.

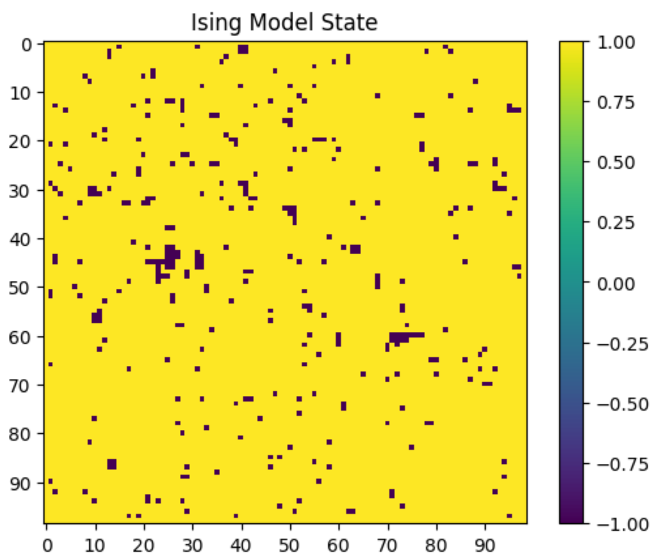
We calculate the probability of keeping the system by checking to see if the change in energy is positive (meaning the new state has higher energy) or negative (meaning the old state has higher energy). If the change in energy is negative the probability of keeping the system is set to 1 which guarantees that the state is kept. If the change is negative the probability is set to:

$$P_a = e^{-\frac{1}{k_b T}\Delta E}$$

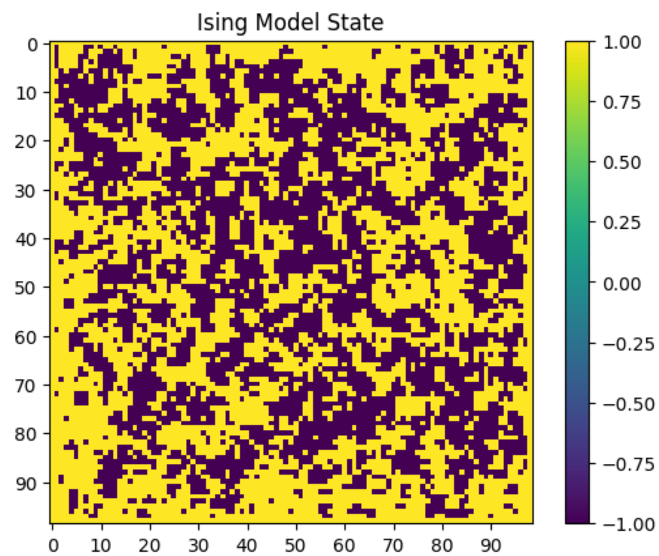
We then pick a random number between 0 and 1. If it is less than P_a, we keep the state and update our magnetism sum. If we don't keep the state, we instead reset the value at the random index and check if we need to reset any of the boundary values. If a changed value is at an edge, the opposite ghost cell will also need to be changed. The steps are then repeated for a set number of times which leads to convergence. The code that runs MCMC is stored in ising.cpp mcmc.h and vary_H.cpp which are all similar, but have slight differences based on what we are looking for.

2.2 2D Ising Model Convergence

Through use of the MCMC method, we obtained a picture of the magnetism patterns of the Ising model which we then can plot to visualize what the states look like. In this case we hope to show the system reaching equilibrium for different temperatures.

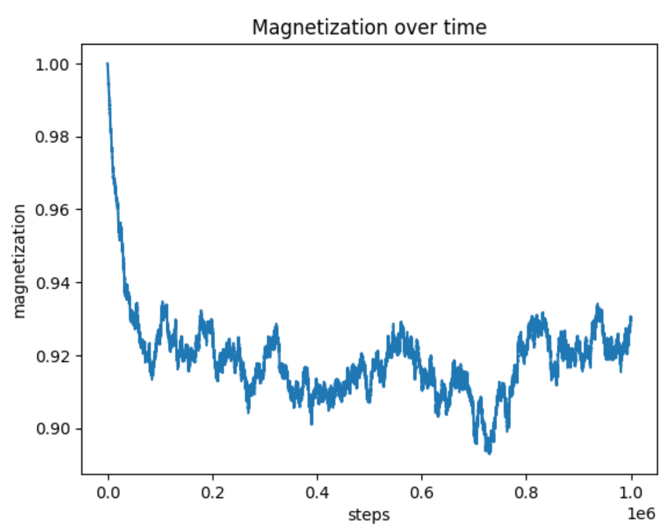


(a) Ising Model State with $k_bT = 2$ and with random seed 209ed0a2c8d8b863.

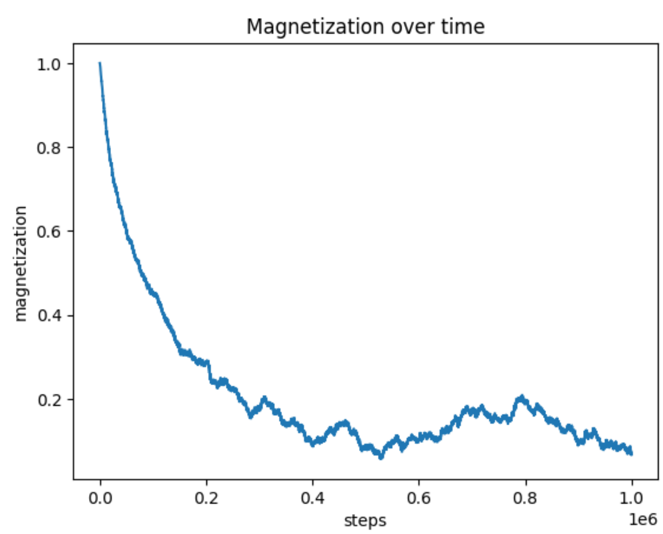


(b) Ising Model State with $k_bT = 3$ and with random seed 1246dccaf20963b9.

When graphing the Ising grid after convergence, we see that at higher temperatures the Ising model converges and reaches equilibrium with a more even spread of -1 and 1 values. These plots were produced with 1,000,000 MCMC steps and a grid size of 100 by 100. The mean magnetization was found specifically by taking the mean only after we were sure we reached equilibrium, so specifically we used the last 5,000 steps.

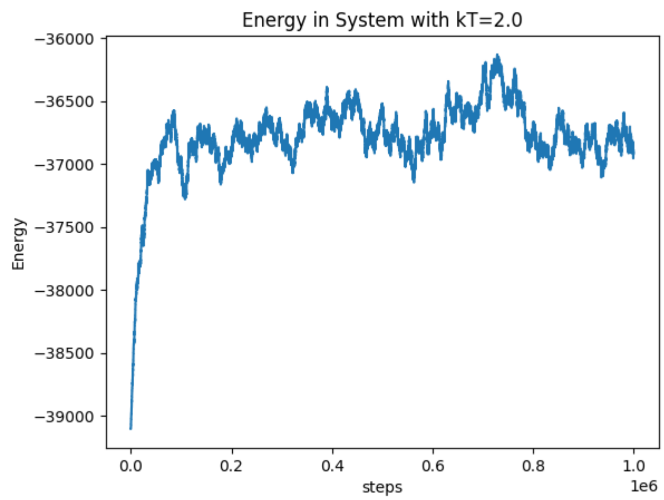


(a) Magnetization over time for $k_bT = 2$ with random seed 209ed0a2c8d8b863. The mean magnetization at end was found to be 0.9222501858800001

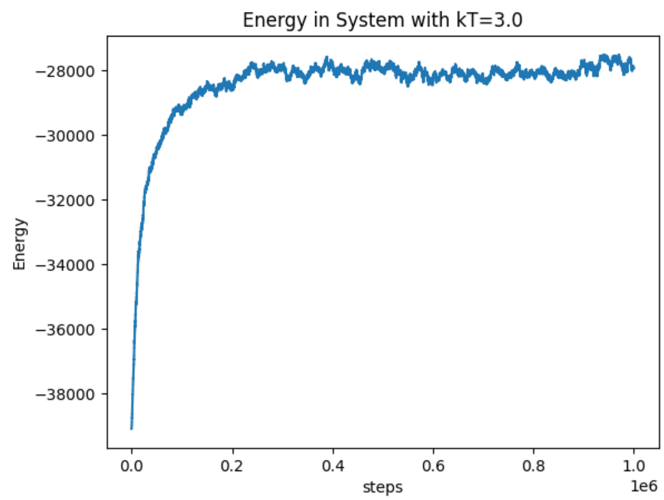


(b) Magnetization over time for $k_bT = 3$ with random seed 1246dccaf20963b9. The mean magnetization at end for was found to be 0.085867625391999999.

Looking at how the magnetization changes over the steps of the MCMC reveals information about it's convergence. Looking at the graphs, it seems that at higher temperatures the steps are more stable and the system converges slightly faster.



(a) The energy over time for $k_bT = 2$ with random seed 209ed0a2c8d8b863.



(b) The energy over time for $k_bT = 3$ with random seed 1246dccaf20963b9.

Not surprisingly, the energy also converges faster at higher temperatures, and is more stable which makes sense as it is dependent on the magnetization. We see that thermal equilibrium is first reached after about 100,000 to 200,000 steps of the MCMC process.

Overall though, the graphs indicate that we can be confident about our implementation of the MCMC process, especially as we take more steps.

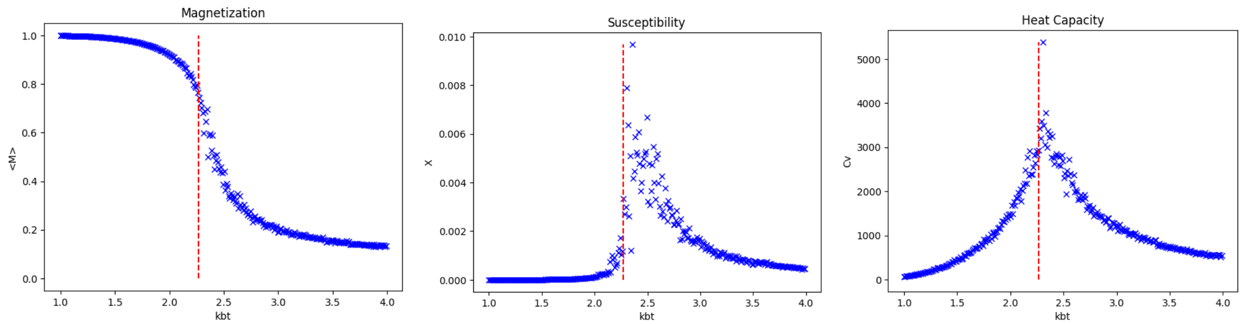
3 Result

3.1 Phase Transition

By calculating the expectation value of the Magnetism and Energy, we then can calculate the magnetic susceptibility and heat capacity. The expectation values were calculated by summing the magnetism and energy values for each state that was kept and dividing by the number of states. To calculate the squared values, the magnetism and energy values were squared before they were summed. The vary_kbt.cpp and mcmc.h were used to generate the data to graph. For each run we used tested across 300 temperatures, ranging between 0.0 and 4.0. With each temperature we did a new MCMC run with a new random seed, preventing any possibility of looping around to the same values. We also ran the MCMC code out to 5,000,000 steps each time and in order to cut down on computation time we only used a 50 by 50 grid.

The values are graphed over a range of temperatures in PhaseTransitionPlot.ipynb, so that we can identify the critical temperature. At the critical temperature we expect the material to instantly lose its permanent magnetic properties, resulting in the magnetization going to 0 and the magnetic susceptibility and heat capacity both diverging.

The theoretical critical temperature should be approximately 2.269J for the Ising model. We initially attempted to find the critical temperature using J=1 producing the images below.



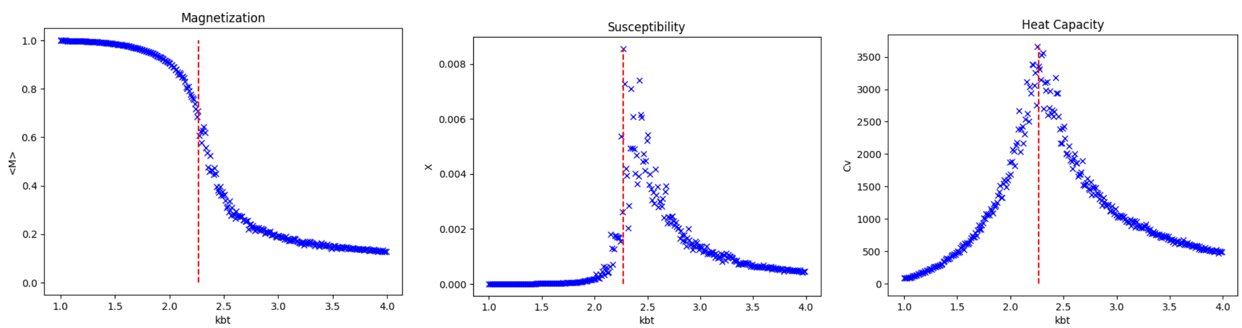
(a) Magnetisation calculated from all kept states with J=1.0. The red line denotes the theoretical critical temperature.

(b) Magnetic susceptibility calculated from all kept states with J=1.0. The red line denotes the theoretical critical temperature.

(c) Heat capacity calculated from all kept states with J=1.0. The red line denotes the theoretical critical temperature.

Due to the imperfect and finite nature of our simulation you will notice that the expected behavior doesn't occur instantaneously, but instead gradually. Additionally, it's clear that the divergence of susceptibility and heat capacity are not perfectly aligned with the theoretical critical temperature. We based the simulated critical temperature based on the temperature at which susceptibility and heat capacity each reach a maximum, which indicates the temperature of maximum divergence. For magnetic susceptibility this value was 2.35452 J, and for heat capacity it was 2.30435 J. These values are a bit off from our expected 2.269 J, so we set out to improve it by modifying J.

We are able to get more accurate results when using a values of J = 0.975 when running MCMC.



(a) Magnetisation calculated from all kept states with J=0.975.

(b) Magnetic susceptibility calculated from all kept states with J=0.975.

(c) Heat capacity calculated from all kept states with J=0.975.

Based on this run for susceptibility we found a critical temperature of 2.27425 J, and for heat capacity we found it to be 2.25418 J. These values are much closer to the theoretical value and also visually agree well with the graphed expected value. It's interesting to note how altering J shifts the graphs forwards or backwards, although it makes sense as the energy is proportional to J.

3.2 Magnetic Hysteresis

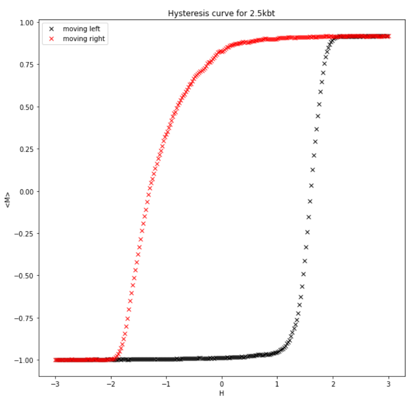
For this section, we introduce an external magnetic field H. This magnetic field can either add to or compete with the magnetization caused by the first term. The effect on the Hamiltonian can be represented as follows:

$$H = -J\sum \sigma_a \sigma_b - H \sum \sigma_a$$

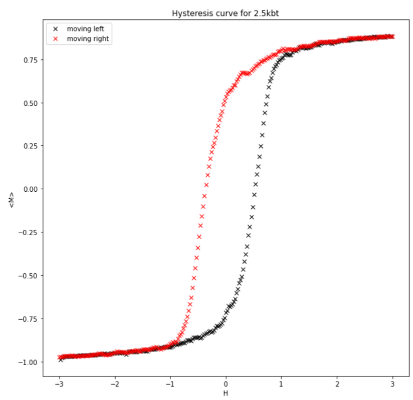
.

The goal of this exercise is to realize hysteresis curves in the relationship between H and $< M >$. Assume we have a strong initial state, such that all states are aligned against the magnetic field. As we decrease the field, and eventually flip it to positive, there will be an initial resistance from the state's magnetism. Only at a certain strength of H will the $< M >$ flip. This relationship is known as the "Hysteresis Curve." We attempt to realize the relationship between H and $< M >$ for different values of $k_B T$.

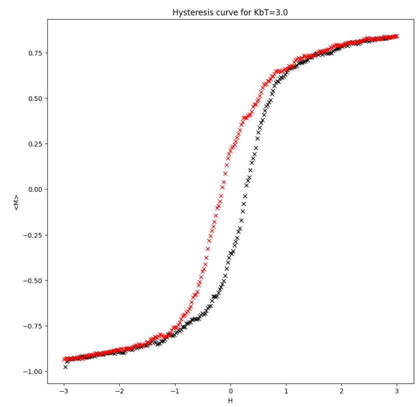
Contrary to the method given, we began with all states aligned opposite to the field, instead of aligned with it. 5,000,000 MCMC steps were taken, with the H of the field being varied every 10,000 steps. Averages were taken over every constant H frame. We started at H=-3, traveled to H=3, and then back to H = -3, completing a full loop. Different graph colors were used to describe the different paths.



(a) Hysteresis Plot with $k_B T = 1.5$



(b) Hysteresis Plot with $k_B T = 2.5$



(c) Hysteresis Plot with $k_B T = 3.0$

From the provided graphs, we observe that the delay for the flip of magnetization is longer for higher temperatures. This patterns appears in both directions. This is as expected for a hysteresis curve. Within our hysteresis plots you can also see that variance seems to increase as our temperature increases.

4 Error & Conclusion

As seen with the 2D Ising model, the MCMC method is incredibly sensitive to the number of steps used. If you don't allow it to run for enough steps it won't fully converge and will be slightly inaccurate. Additionally, because on average you are taking over 1,000,000 steps, while a singular MCMC run isn't too computationally intensive, multiple can take a while.

In terms of our calculation of phase transition temperature, we recognize that simply taking the maximum values of susceptibility and heat capacity isn't a full proof method, and so there's some error involved. Additionally, for both our finding of critical temperature and our graphing of magnetic hysteresis we used a limited number of values within the respective temperature ranges and only had grid sizes of 50 by 50 which introduces inherent limitations on accuracy. In addition, our method for averaging and our initial state in the magnetic hysteresis test also could introduce some variance from other produced results.

Our procedure also utilizes random numbers which introduces an inherent risk of error and some difficulty with repeatability of our exact results, however overall trends and approximate answers can still be trusted.

Overall, we were still able to succesfully implement the MCMC method to simulate a 2D Ising model and use it as a tool for exploring the behavior of ferromagnets.