2D Ising Model with MCMC

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The 2D Ising model is a powerful tool in statistical mechanics which allows us to represent the behavior of ferromagnetic materials. In this project, we use Markov Chain Monte Carlo (MCMC) techniques, specifically the Metropolis-Hastings algorithm, to simulate the 2D Ising model. We discuss our decisions for the various parameters for the MCMC simulation such as thinning and number of burn-in steps. By varying several properties such as magnetic field strength and temperature, we gain insights on the behavior of the system, including phase transitions. Our results demonstrate phase transitions at the Curie temperature as well as the relationship between magnetization, temperature, and magnetic field strength. We also discuss optimizations to our code. Through this project, we increase our understanding of ferromagnetism and MCMC processes.

I. INTRODUCTION

The 2D Ising model is a physical model used to describe ferromagnetism in statistical mechanics. It consists of a grid-like square lattice where each cell in the lattice has a magnetic moment (spin) that can be either up $(+1)$ or down (-1). An example of one such Ising model can be seen in Figure 1. The 2D Ising model allows for the analysis of phase transitions at zero external magnetic field within a simplistic framework, illustrating how local interactions can lead to collective behavior [1]. By applying the external field to the model, we are also able to study the relationship between magnetization of the system, magnetic field, and temperature.

There are many ways to simulate the 2D Ising model, but we use Markov Chain Monte Carlo (MCMC) techniques to try to visualize the underlying physical principles. A Markov Process gives us probabilistic rules to transition through a system where the next state depends solely on the current state. Repeatedly applying the Markov process moves the system through a "random sequence" of states, forming a Markov Chain.

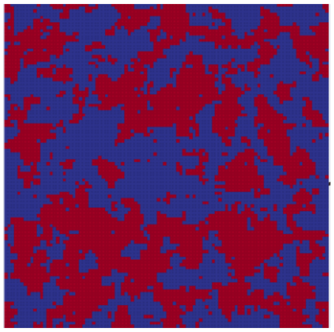

FIG. 1. 2D Ising Model; blue indicates negative spin while red represents positive.

The "random sequences" should not be truly random, since you want to simulate physically probable situations. The Monte Carlo method addresses this issue through the introduction of random sampling. This allows for the estimation of probabilities and behaviors of the Ising model without needing to examine every single possibility.

The MCMC method uses both of these strategies by using Monte Carlo processes, in our case the Metropolis-Hastings algorithm, to generate long Markov chains. Using this, one can calculate moving averages of various quantities, which converge to their true probabilistic values for long enough chains.

The Metropolis-Hastings algorithm [2] works by comparing a given state with another random state and deciding to accept or reject the result based on certain considerations. The Metropolis-Hastings algorithm also ensures that a simulation behaves correctly, maintaining a "detailed balance". This equilibrium requires that the rate of transition from any state to its successor and vice versa remains invariant. This balance helps us achieve a stable, consistent distribution of states that reflects the true nature of the 2D Ising model [3].

In the context of the 2D Ising model, MCMC simulations help visualize and understand the equilibrium and dynamical properties of the system. These techniques allow for the estimation of physical quantities, such as magnetization and susceptibility, by simulating the state of the system over time and analyzing the resulting data [4].

Our code can be accessed via the group's GitHub [5]. As we will discuss later, it can be run the standard way through python or the speed optimized way using C++.

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II. METHODS

A. Equations

Simulation of the 2D Ising model requires two main formulae: the magnetization of the system and the energy of spin configuration.

$$M(\sigma) = \frac{1}{|\Lambda|} \sum_{i \in \Lambda} \sigma_i \tag{1}$$

Equation 1 allows us to calculate the average magnetic moment per lattice site in the 2D Ising model. Summing up the spins across all lattice sites and dividing by the total number of sites yields magnetization M. Λ refers to the lattice and $|\Lambda|$ refers to the number of lattice sites, while σ_i refers to the spin at lattice site i.

$$E(\sigma) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - B \sum_{i \in \Lambda} \sigma_i \tag{2}$$

Equation 2 quantifies the system's total energy, comprising of two parts: interaction energy between adjacent spins and energy due to an external magnetic field B. In the first part, the sum of the product of neighboring spin pairs multiplied by the spin-spin interaction J indicates energy preference for aligned or opposite spins. The term $\langle ij \rangle$ represents two adjacent sites i and j. J is set to be constant for vertical and horizontal spins signifying the isotropic case for the 2D Ising model. In the second term, the sum of spins over all sites multiplied by B reflects the field's influence on spin alignment. Negative signs in both terms denote energy minimization when spins align with each other and the external field for ferromagnetic coupling ($J > 0$). Along with the formulae above, in order to study and describe the behavior of the system at different temperatures, it is useful to know the critical temperature at which we expect the phase transitions.

$$T_c K_b / J = 2/ln(1 + \sqrt{2}) \approx 2.269 \tag{3}$$

Equation 3 approximates the critical temperature for the 2D Ising model, also known as Curie point [6]. J is the spin-spin interaction, K_b is Boltzmann's constant, and T_c is the critical temperature. This formula works for the isotropic case in which horizontal and vertical J are set to equal each other. The critical temperature marks the transformation of the material from ferromagnetic to paramagnetic. We can then set a range of temperature values below and above the point to observe phase transitions, as well as the behavior of the system when the material is ferromagnetic or paramagnetic.

B. Code

The code implements the Metropolis-Hastings algorithm for an MCMC simulation of the 2D Ising model. This algorithm proceeds as follows: first, choose a random point within the lattice; second, compute the change in energy associated with flipping the spin at that point; third, decide weather or not to flip the spin at that point. This process is repeated many times as the system converges. We can then use the converged system (post burn-in) to compute the mean magnetization.

The first step requires use of a random number generator to select a single lattice point. We then access the neighboring points, and the external magnetic field to compute the change in energy associated with flipping the spin of this, random point. If the change in energy is negative, we accept the change and update the lattice to flip the point in question. If the change in energy is positive, we decide using Metropolis-Hastings. This means the change is accepted with a probability proportional to the magnitude of the change in energy and to the temperature. The temperature dependency makes the system more random for high temperatures; a point is more likely to flip compared to its neighbors, or against the magnetic field at high temperature.

We made three implications of the core algorithm. The first two were in python, one vectored and the other conventional. The performance gain for vectorization was minimal, and the memory usage was prohibitive at the full 100x100 lattice size. To address this, we used pybind11 to re implement the conventional version in C++ with a Python wrapper. The performance gain was about 50x in C++ compared to Python, however pybind11 causes platform dependencies which mean it only runs on a system with which it is compiled. This prevented us from packaging it with our final implementation, but the code is included in the repository. It is also wrapped in the utils.py script.

A key optimization that was made across all implementations was the vectorization of the calculation of mean energy in the lattice. We recognized that, for any given simulation step, the lattice spins can change at only one point. By calculating the initial total spin, we can update a list of total spins for each step using one addition operation (if a spin is changed). At the end of the simulation, we calculated the mean total energy by dividing the list of total energies by the size of the lattice. That prevents calling np.mean on each step, which would otherwise perform 100x100 addition operations per step.

The pseudo-code in Algorithm 1 shows our implementation of MCMC with Metropolis-Hastings algorithm. Lines 1-7 initialize the lattice. Lines 8-14 are the loop for each MCMC step (Lines 11-13 encapsulate the Metropolis-Hastings algorithm). Line 16 returns the simulation results.

C. Parameters

The algorithm also requires the definition of a few parameters including the initial configuration, burn-in steps, total steps, and thinning.

Algorithm1 Simplified Pseudocode for 2D Ising Model Simulation

```
Initialize simulation parameters: steps, temperature, lattice size, etc.
if starting with random spin configuration then
    Initialize lattice with random spins
else
    Initialize lattice with all spins up
end if
Initialize an array to store magnetization values
for each step in the simulation do
    Randomly select a lattice site
    Compute the change in energy for flipping the spin at this site
    if the spin flip lowers the energy or meets the acceptance probability ($\propto \Delta E^{-1}$) then
        Flip the spin at the selected site
    end if
    Update and record the magnetization
end for
Output the magnetization values and final spin configuration
```

[1]

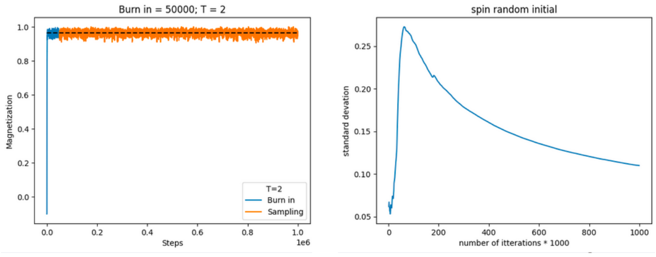


FIG. 2. Burn-In Steps

1. *The Initial Configuration*

The initial configuration of the system has two main types: aligned spins, where all spins are in the same direction, or randomized spins with equal probability. Both configurations have their advantages depending on the purpose of the simulation. For studying the behavior of the system at the phase transitions, the randomized initial configuration is more suitable. This type of initial configuration represents a more disordered state of the system, which is better for studying the behavior near phase transition. It captures the influence of thermal fluctuations on the system at higher temperatures, and thus the critical point. Aligned spins initialization would take longer to account for these fluctuations since it is mainly used for studying ferromagnetic materials (at low temperatures).

2. *Burn-In Steps*

In order to get the most probable results from our simulation, we discard the initial behavior of the system from before it nears equilibrium. These initial discarded steps are called burn-in steps. There are various approaches to determine the optimal number of steps to burn in. Our solution was to analyze the relationship between standard deviation of magnetization and step number, shown in Figure 2. We see that for later steps, the standard deviation follows the pattern we expect to see for error in an MCMC simulation. However, we notice a critical point near the start of the graph, where standard deviation is greatly varied from the expected relation. We choose to burn in steps prior to this critical point. Based on our analysis, the burn-in value we used was 350,000 steps.

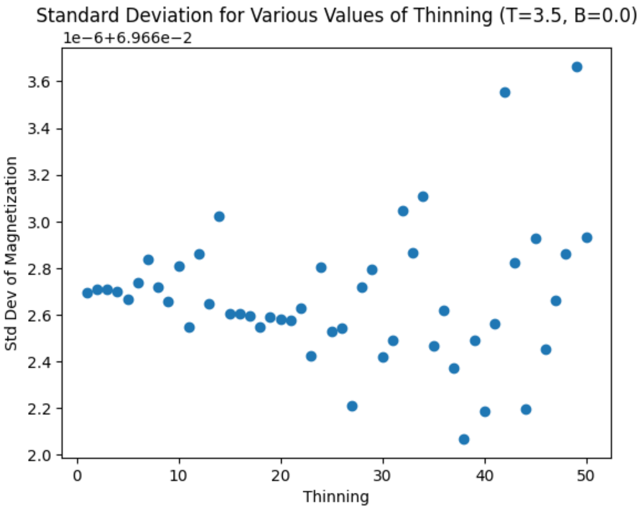


FIG. 3. Standard Deviation for Thinning

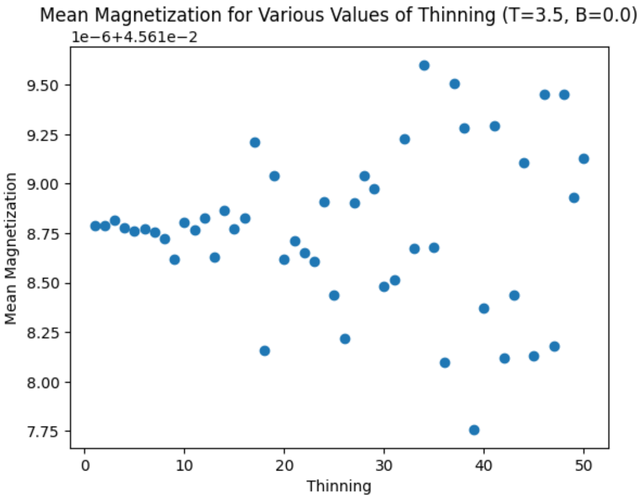


FIG. 4. Mean Magnetization for Thinning

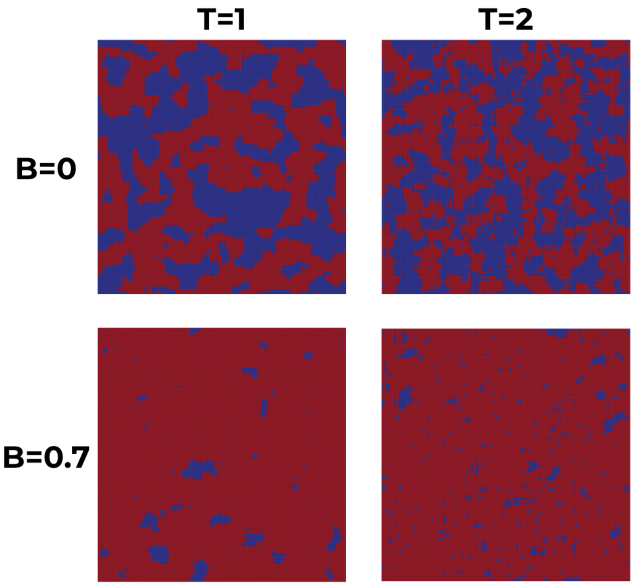


FIG. 5. Effects of Temperature and External Magnetic Field

3. Thinning

Thinning in MCMC refers to the process of selecting only every nth value in the chain in order to make the data points independent from one another. To determine the optimal amount of thinning to use, we plot results for a single simulation of 10,000,000 steps, thinned by values from 1 to 50. If we saw the mean and standard deviation values trending as thinning increased, then we would conclude that thinning improves the results. However, as seen in 4 and 3, we observe that the values of both the mean and standard deviation are just as likely to increase or decrease. This results is consistent with simply having fewer data points. Based on our analysis, we decided that thinning is unnecessary for our purposes.

4. Total Steps

Since we know our MCMC will converge closer to the expected value for larger numbers of steps, we want the largest number of total steps which is computationally viable to maximize accuracy. With our final optimized code, we were able to easily compute 1,000,000 steps. In practice, our results and analyses are the product of runs between 2 and 10 million steps.

III. RESULTS

The 2D Ising model at different temperatures T and magnetic field strengths generated using MCMC and the Metropolis-Hastings algorithm can be seen in Figure 5. For increased temperature, the Ising model is more disordered as a result of increased thermal fluctuations. For increased magnetic field, we see more spin alignment in the Ising model, which clearly lines up with the theoretical result.

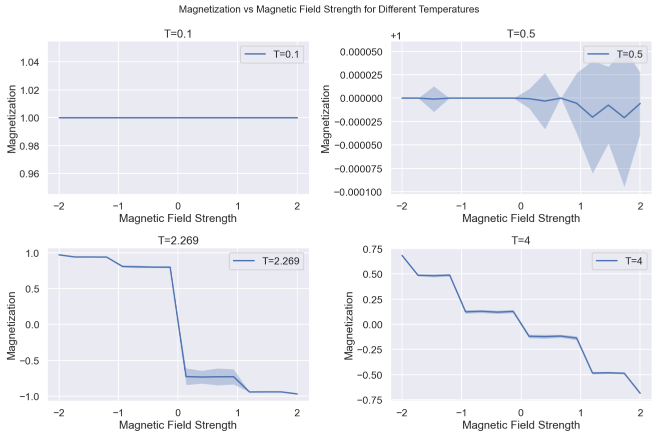


FIG. 6. Magnetization vs Magnetic Field Strength for Different Temperatures

1D plots of magnetization versus magnetic field for different temperatures are shown in Figure 6. We plot magnetization as a function of changing magnetic field for values of temperature that are below, at, or above critical temperature to observe the behavior of the system.

For low temperatures, below the Curie point, the magnetization of the system does not change as external field strength is increased. At low temperature, the system experiences quantum effects rather than classical. Thus, the thermal fluctuations have less influence on the system and the magnetic field does not have a large affect on the magnetization.

For the critical temperature, the plot shows a first order phase transition when there is no present external field. A first order phase transition is an abrupt change of the state of the system. It happens at the critical temperature because this is where the system becomes highly affected by the thermal fluctuations, thus the change in the magnetic field causes a spontaneous change in the magnetization direction.

Above the critical temperature, magnetization starts behaving proportionally to the magnetic field strength. It decreases to zero as magnetic field decreases, and then increases as the magnetic field increases. The change in the magnetic field makes the magnetization flip a sign. At high temperatures, the system is dominated by the thermal fluctuations, so we expect the magnetization to be fully dependent on the changing magnetic field.

The 1D plots of magnetization versus temperature for different magnetic fields can be seen in Figure 7. In these plots, the strength of the external magnetic field is fixed and magnetization is varied as a function of temperature for negative, positive and the zero external field. For a negative magnetic field, the system continuously loses

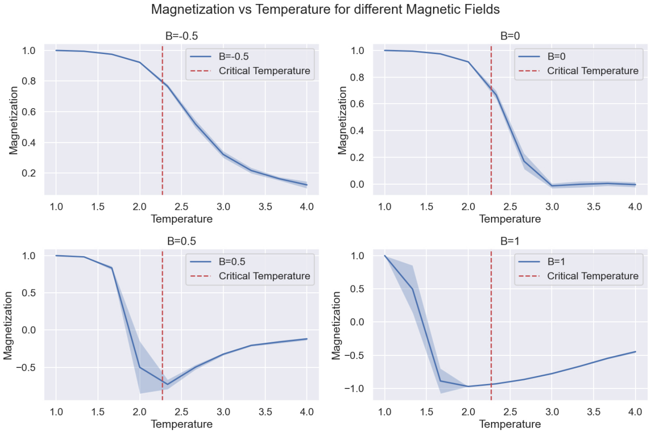
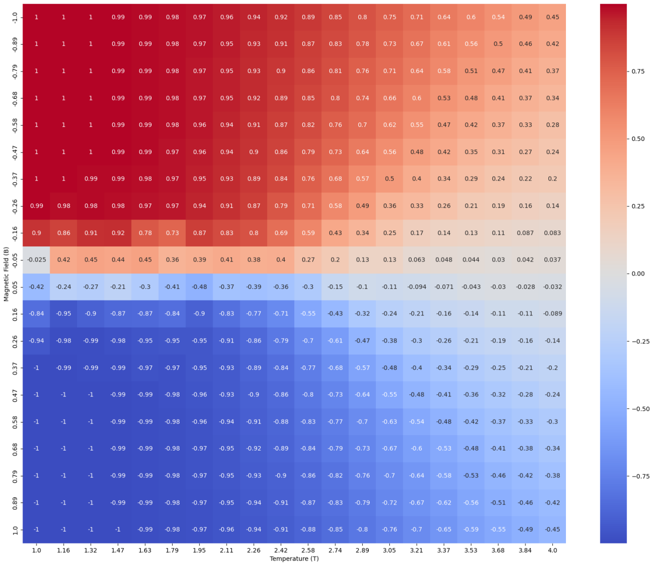


FIG. 7. Magnetization vs Temperature for Different Magnetic Fields



	1.0	1.16	1.32	1.47	1.63	1.79	1.95	2.11	2.26	2.42	2.58	2.74	2.89	3.05	3.21	3.37	3.53	3.68	3.84	4.0
-1.0	1	1	1	0.99	0.99	0.98	0.97	0.96	0.94	0.92	0.89	0.85	0.8	0.75	0.71	0.64	0.6	0.54	0.49	0.45
-0.89	1	1	1	0.99	0.99	0.98	0.97	0.95	0.93	0.91	0.87	0.83	0.78	0.73	0.67	0.61	0.56	0.5	0.46	0.42
-0.79	1	1	1	0.99	0.99	0.98	0.97	0.95	0.93	0.9	0.86	0.81	0.76	0.71	0.64	0.58	0.51	0.47	0.41	0.37
-0.68	1	1	1	0.99	0.99	0.98	0.97	0.95	0.92	0.89	0.85	0.8	0.74	0.66	0.6	0.53	0.48	0.41	0.37	0.34
-0.58	1	1	1	0.99	0.99	0.98	0.96	0.94	0.91	0.87	0.82	0.76	0.7	0.62	0.55	0.47	0.42	0.37	0.33	0.28
-0.47	1	1	1	0.99	0.99	0.97	0.96	0.94	0.9	0.86	0.79	0.73	0.64	0.56	0.48	0.42	0.35	0.31	0.27	0.24
-0.37	1	1	0.99	0.99	0.98	0.97	0.95	0.93	0.89	0.84	0.76	0.68	0.57	0.5	0.4	0.34	0.29	0.24	0.22	0.2
-0.26	0.99	0.98	0.98	0.98	0.97	0.97	0.94	0.91	0.87	0.79	0.71	0.58	0.49	0.36	0.33	0.26	0.21	0.19	0.16	0.14
-0.16	0.9	0.86	0.91	0.92	0.78	0.73	0.87	0.83	0.8	0.69	0.59	0.43	0.34	0.25	0.17	0.14	0.13	0.11	0.087	0.083
-0.05	-0.025	0.42	0.45	0.44	0.45	0.36	0.39	0.41	0.38	0.4	0.27	0.2	0.13	0.13	0.063	0.048	0.044	0.03	0.042	0.037
0.05	-0.42	-0.24	-0.27	-0.21	-0.3	-0.41	-0.48	-0.37	-0.39	-0.36	-0.3	-0.15	-0.1	-0.11	-0.094	-0.071	-0.043	-0.03	-0.028	-0.032
0.16	-0.84	-0.95	-0.9	-0.87	-0.87	-0.84	-0.9	-0.83	-0.77	-0.71	-0.55	-0.43	-0.32	-0.24	-0.21	-0.16	-0.14	-0.11	-0.11	-0.089
0.26	-0.94	-0.98	-0.99	-0.98	-0.95	-0.95	-0.95	-0.91	-0.86	-0.79	-0.7	-0.61	-0.47	-0.38	-0.3	-0.26	-0.21	-0.19	-0.16	-0.14
0.37	-1	-0.99	-0.99	-0.99	-0.97	-0.97	-0.95	-0.93	-0.89	-0.84	-0.77	-0.68	-0.57	-0.48	-0.4	-0.34	-0.29	-0.25	-0.21	-0.2
0.47	-1	-1	-1	-0.99	-0.99	-0.98	-0.96	-0.93	-0.9	-0.86	-0.8	-0.73	-0.64	-0.55	-0.48	-0.41	-0.36	-0.32	-0.28	-0.24
0.58	-1	-1	-1	-0.99	-0.99	-0.98	-0.96	-0.94	-0.91	-0.88	-0.83	-0.77	-0.7	-0.63	-0.54	-0.48	-0.42	-0.37	-0.33	-0.3
0.68	-1	-1	-1	-0.99	-0.99	-0.98	-0.97	-0.95	-0.92	-0.89	-0.84	-0.79	-0.73	-0.67	-0.6	-0.53	-0.48	-0.41	-0.38	-0.34
0.79	-1	-1	-1	-0.99	-0.99	-0.98	-0.97	-0.95	-0.93	-0.9	-0.86	-0.82	-0.76	-0.7	-0.64	-0.58	-0.53	-0.46	-0.42	-0.38
0.89	-1	-1	-1	-0.99	-0.99	-0.98	-0.97	-0.95	-0.94	-0.91	-0.87	-0.83	-0.79	-0.72	-0.67	-0.62	-0.56	-0.51	-0.46	-0.42
1.0	-1	-1	-1	-1	-0.99	-0.98	-0.97	-0.96	-0.94	-0.91	-0.88	-0.85	-0.8	-0.76	-0.7	-0.65	-0.59	-0.55	-0.49	-0.45

FIG. 8. Phase Diagram in T vs. B of the 2D Ising Model

its magnetic properties as the temperature increases and reaches the critical point. For the absence of the external magnetic field, a more spontaneous phase transition is apparent, where the system goes from ferromagnetic to paramagnetic state. The system also becomes fully demagnetized. For a positive magnetic field, the magnetization undergoes a first order phase transition and flips its sign, then continuing to decrease as the temperature reaches the critical value.

In both sets of plots, Figure 6 and Figure 7, hysteresis can be observed. Hysteresis is the phenomenon that describes the system's dependence on its past history, rather than only its current conditions, such as temperature or applied external field. In the graphs, this behavior of the system is indirectly represented through the coexistence region between ordered and disordered phases. For the phase transitions in Figure 7 (positive fixed magnetic field), we can observe the state of the system for different magnetization values with the same magnetic field and temperature. This signifies that for a certain value of temperature and magnetic field, the system can have different magnetization values depending on its previous history.

The phase plot of the magnetization verse temperature can be seen in Figure 8. We accomplish this by making a heat map of the average magnetization after the burn in phase at each temperature and external field point. Each cell was trained for 1 million steps to ensure that it reached an equilibrium state. When temperature approaches absolute zero, the system reaches a ground state where all spins align in the direction of the external field (if present) or in one direction spontaneously. This can clearly be seen by the bright red and blue at the top and and bottom of the plot.

When there is no magnetic field, we see the same result we saw for homework 3. The system's response to an external magnetic field, quantified by the magnetic susceptibility, diverges after the temperature is above the critical point. This means that the net magnetization is around 0.

However having a nonzero magnetic field breaks this symmetry. Even at temperatures greater than the critical point, where the system would normally be in a disordered state, the external field can induce a net magnetization. This breaking of symmetry is what makes 2D Ising models so complicated and requires them to be simulated rather than calculated.

IV. CONCLUSION

In this project, we successfully implemented a MCMC simulation to study the 2D Ising model, significantly advancing our understanding of ferromagnetism in statistical mechanics. Utilizing the Metropolis-Hastings algorithm allowed us to visualize and analyze the equilibrium and dynamical properties of ferromagnetic materials under various conditions. One of the key achievements was the integration of C++ for computationally intensive parts of our code, which substantially reduced runtime and enhanced our simulation capabilities.

However, we learned that while implementing C++ accelerates computation, it complicates the setup for other users, and obstacle we did not expect to face. This shows the importance of balancing high-performance computing with ease of use and comprehensive documentation.

Looking ahead, we are curious to explore how these simulations translate to real-world phenomena and to test their applicability in practical scenarios involving ferromagnetic materials. Additionally, we plan to investigate alternative computational methods, such as variational autoencoders [7] to model 2D Ising systems. These methods promise faster processing and the ability to handle more complex situations, although they also present challenges in terms of reliability and training.

V. CONTRIBUTIONS

All team members significantly contributed to writing the code, creating the presentation, and creating the final paper. Additional contributions are listed:

Dmitri Demler did significant work on generating the phase diagram.

Anastasiia Lishchenko did substantive research contributing to theoretical understanding of topics such as first order phase transitions.

Leo Megliola worked to optimize the MCMC process using C++.

Zachary Sherman provided significant proofreading and formatting of the presentation and paper.

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