UNIVERSITY OF NOTRE DAME

Simulating the Ising Model using the Metropolis-Hastings Algorithm

Isaiah Mumaw

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1 INTRODUCTION

The Ising model is a statistical mechanical model of ferromagnetism, a property which allows certain materials to retain magnetization after being exposed to a magnetic field. In this model, the spins are given by $s_i = \pm 1$, and the overall state of the system is given as the set of all spins: $\boldsymbol{S} = \{s_1, \ldots, s_N\}$.

As a ferromagnetic, the spin of each particle is susceptible to a magnetic field. Additionally, they can interact with nearby particles in the system. These electrostatic interactions are assumed to only happen between directly adjacent particles, with all nonadjacent interactions being small enough in real ferromagnets to consider negligible in this model. This model also disregards magnetic interactions, as they are roughly four orders of magnitude smaller than electrostatic interactions [1].

Given the above interactions, the total energy of the Ising Model in one dimension is:

$$E(\boldsymbol{S}) = \mu B \sum_{i=1}^{N} s_i - J \sum_{i=1}^{N} s_i s_{i+1} \tag{1.1}$$

where μ is the magnetic moment of each spin, B is a uniform magnetic field, J is the electrostatic interaction, and the total number of particles is N.

Given the energy, the specific heat of the state $\boldsymbol{S}$ is given as:

$$C(\boldsymbol{S}) = \frac{dE(\boldsymbol{S})}{dT} \tag{1.2}$$

Additionally, the total magnetization is given as the average of all spins in the state $\boldsymbol{S}$:

$$\boldsymbol{M}(\boldsymbol{S}) = \frac{1}{N}\sum_{i=1}^{N} s_i \tag{1.3}$$

And the magnetic susceptibility is given as:

$$\chi(\boldsymbol{S}) = \left.\frac{\partial \boldsymbol{M}(\boldsymbol{S})}{\partial B}\right|_{B=0} \tag{1.4}$$

In higher dimensions, the state ($\boldsymbol{S}$) is converted from a list to a matrix, with corresponding adjustments to other calculations. Fortunately, most of these are trivial, with the exception of Eq. 1.1, which must now account for neighbor interactions in other directions. For a three-dimensional system, which most closely matches the real world, the energy is as follows:

$$E(\boldsymbol{S}) = \mu B \sum_{i,j,k} s_{i,j,k} - J_x \sum_{i,j,k} s_{i,j,k}s_{i+1,j,k} - J_y \sum_{i,j,k} s_{i,j,k}s_{i,j+1,k} - J_z \sum_{i,j,k} s_{i,j,k}s_{i,j,k+1} \tag{1.5}$$

where J_i describes the electrostatic interaction along each dimension, with all other constants being the same as in the one dimensional model. In the isotropic case, neighbor interactions are equally weighted for each dimension, so all values of J_i are equal. However, in the anistropic case, these values may be different along each direction, resulting in unequal weighting for neighboring interactions.

2 Code Outline

This code was written using the Metropolis-Hastings algorithm, which is a type of Monte Carlo algorithm. In general, this algorithm is used to generate a set of random samples based on a given probability distribution [2].

First, the code generates a random array of up and down spins using numpy.random.choice(), with shape (x,y,z) and with equal weighting given to each spin. This is the initial state of the system.

The algorithm then cycles through each element in the state array. For each step, it calculates the energy of the current state, as well as the energy if the spin of the current particle were flipped. The energies are calculated according to Eq. 1.5. Note that the neighbor interactions are calculated using numpy.roll() along each axis, which allows the code to be applied to arbitrary numbers of dimensions. This also allows for periodic boundaries, as the roll function moves the last row/column into the first position.

The difference between these energies is then sent to the Boltzmann probability equation, given as:

$$P(\boldsymbol{S}) = e^{-E(\boldsymbol{S})/k_B T} \tag{2.1}$$

The resulting probability is compared to a random number between 0 and 1. If the random number is less than the probability, the state is flipped. Otherwise, the state is unchanged. For cases where the resulting change in energy is negative, this flip is guaranteed, as this state is more stable than the original state.

This process is repeated over the entire state array many times in order to reach the equilibrium state.

3 Results

This report analyzes 4 separate types of cases, 3 of which have well-established solutions.

In case 1, an electrostatically interacting system is placed in a field, i.e. $B = J = 1$. In case 2, the interactions are removed ($J = 0$, $B = 1$), and in case 3, the field is removed ($J = 1$, $B = 0$). Finally, case 4 explores the anisotropic Ising model, where J varies for different dimensions. In this case, I have set the x-axis interactions to be extremely strong, while y and z interactions are relatively weak $J = (10000, 1, 1)$. B is set to 0 for this case. In all cases, $\mu = k_B = 1$.

3.1 Magnetization over Time

The first test uses Eq. 1.3 to find the magnetization at each step in the algorithm. Each test is repeated 10 times, with the results averaged. Equilibrium is established when the magnetization stabilizes at a certain value for the majority of trials. These tests were performed at $T = 0$ so as to remove any random thermal fluctuations away from equilibrium, and the initial state was randomly aligned. The results for cases 1 and 2 are shown in Fig. 3.1.

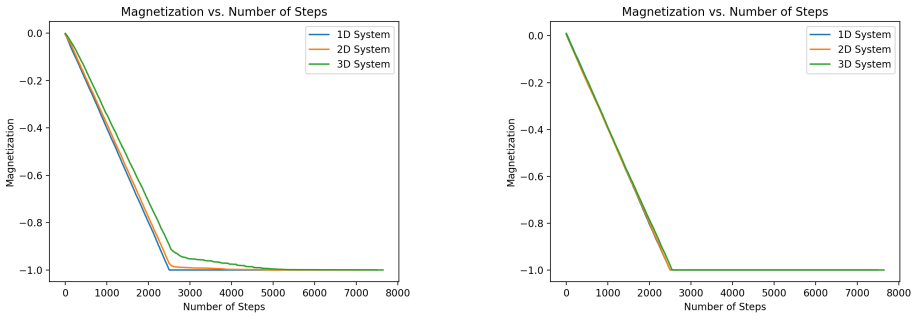

Figure 3.1
Magnetization over time for case 1 (left) and case 2 (right) with randomized initial states at $T = 0$.

If adjusting the initial state, the equilibrium state may be modified. Fig. 3.2 shows the magnetization over time for 75% and 90% up-spins in the initial state for case 1. For a significant proportional of up-spins, the equilibrium state is shifted from entirely down-spin to entirely up-spin.

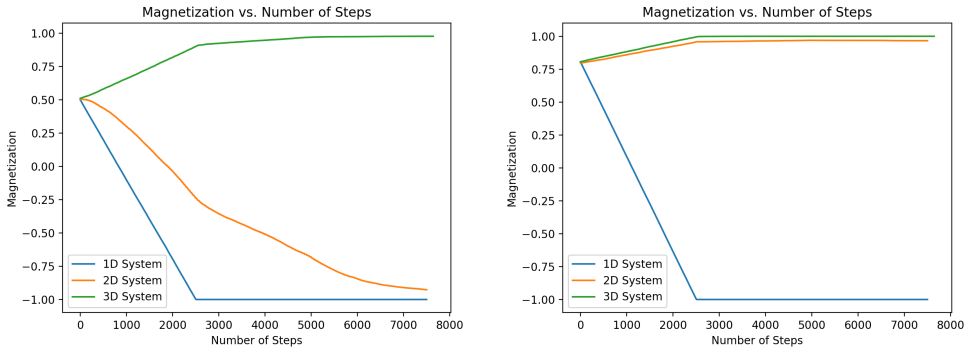

Figure 3.2
Magnetization over time for case 1 with 75% (left) and 90% (right) initial up-spin particles at $T = 0$.

Case 2 had no change regardless of initial state.

The magnetization over time for case 3 is shown in Fig. 3.3.

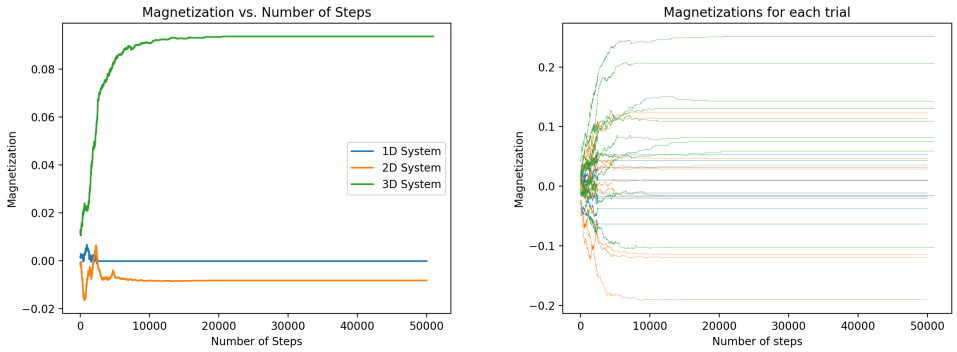

Figure 3.3
Average magnetization over time for 10 trials (left), and the magnetization over time of each trial (right) for case 3. Initial state is randomized, and $T = 0$.

Note that unlike cases 1 and 2, this case does not reach equilibrium, but rather forms regions of like spins, known as domains. These domains are shown in Fig. 3.4, both for the two and three dimensional case.

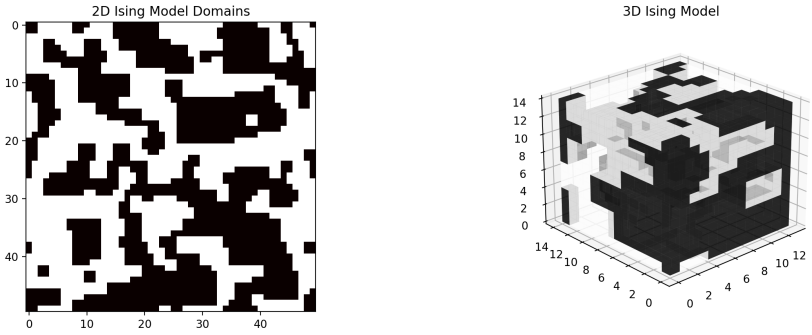

Figure 3.4
Example of domains formed in case 3 for two dimensions (left) and three dimensions (right)

These domains can be corrected for by favoring one spin direction in the initial state (adjusting the p value in numpy.random.choice). The magnetization over time for initial states with 75% and 90% up spins is shown in Fig. 3.5.

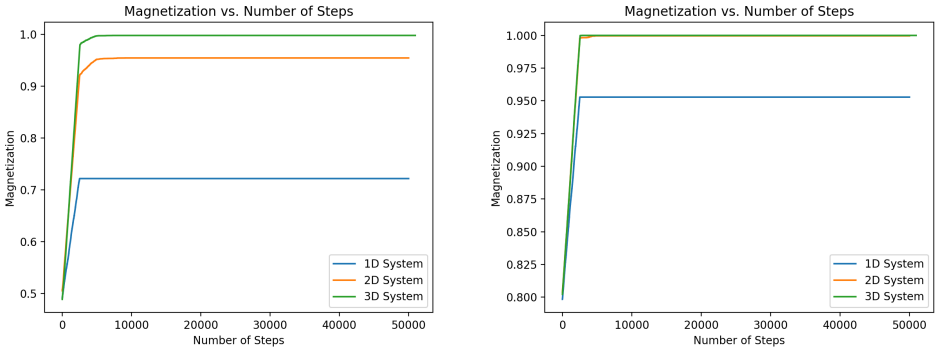

Figure 3.5
Magnetization over time for case 3 with 75% (left) and 90% (right) initial up-spin particles at $T = 0$.

In case 4, only the three-dimensional Ising model is relevant. As with case 3, it forms domains, so Fig. 3.6 shows the magnetization over time in 3 dimensions for 50%, 75%, and 90% up-spins in the initial states. Fig. 3.7 shows the domains in each direction. Note that along the x-direction (front right to back left face), the domains are longer than they are in other directions. This is the effect of the anistropic setup.

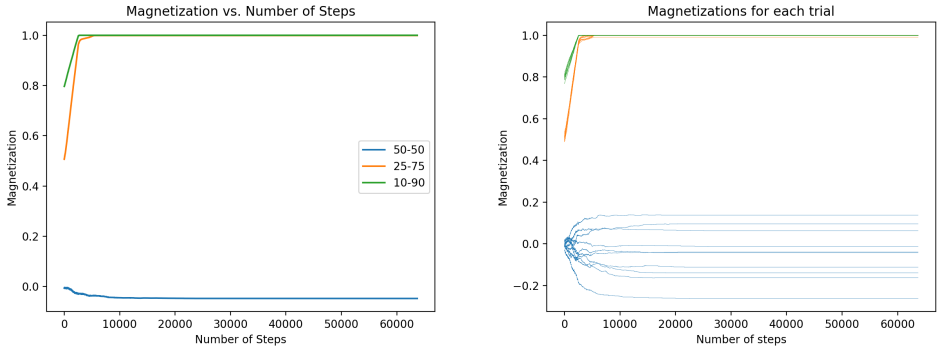

Figure 3.6
Magnetization versus time for case 4, with various initial configurations. The left figure shows the average results, the right figure shows the results per trial.

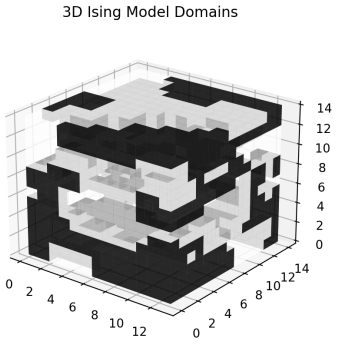

Figure 3.7
Domains formed in case 4

3.2 Magnetization and Susceptibility vs. Temperature

The second set of tests first used Eq. 1.3 while varying the temperature. The magnetization is found by averaging over the values of this equation after reaching equilbrium (based on the results from the previous test). In order to get the magnetic susceptibility, the value of B is reduced by 0.5, and the magnetization test is repeated. The susceptibility is then given by Eq. 1.4.

The magnetization and susceptibility versus temperature for case 1 are given in Fig. 3.8. Note that the magnetization plot also includes the theoretical magnetization, given by the following:

$$\boldsymbol{M}_{\text{theoretical}} = \tanh\left(\frac{\mu B}{k_b T}\right) \tag{3.1}$$

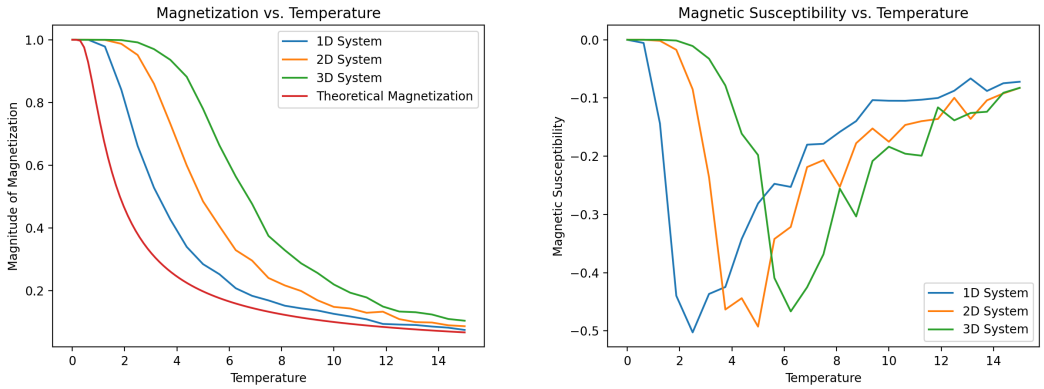

Figure 3.8
Magnetization (left) and susceptibility (right) plotted against temperature for case 1.

The magnetization and susceptibility versus temperature for case 2 are given in Fig. 3.9. The magnetization plot here also includes the same theoretical calculation as in case 1.

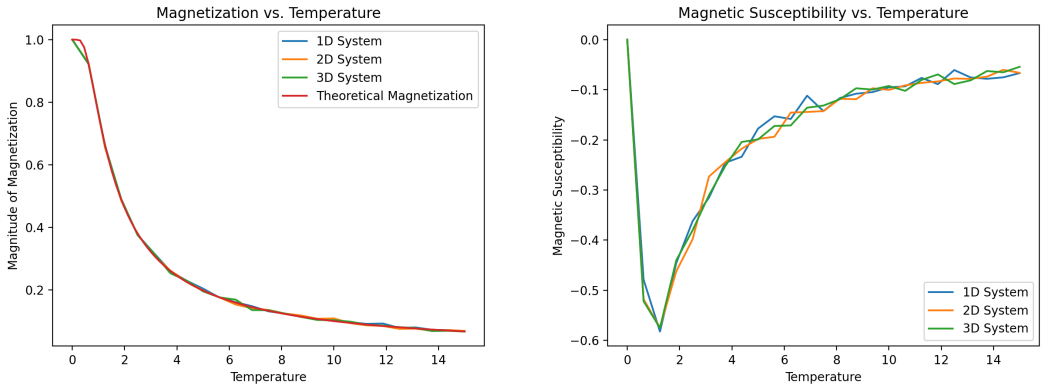

Figure 3.9
Magnetization (left) and susceptibility (right) plotted against temperature for case 2.

The magnetization and susceptibility versus temperature for case 3 are given in Fig. 3.10. The initial state is set to 90% up spins, since this very nearly reaches true equilibrium in the low temperature limit.

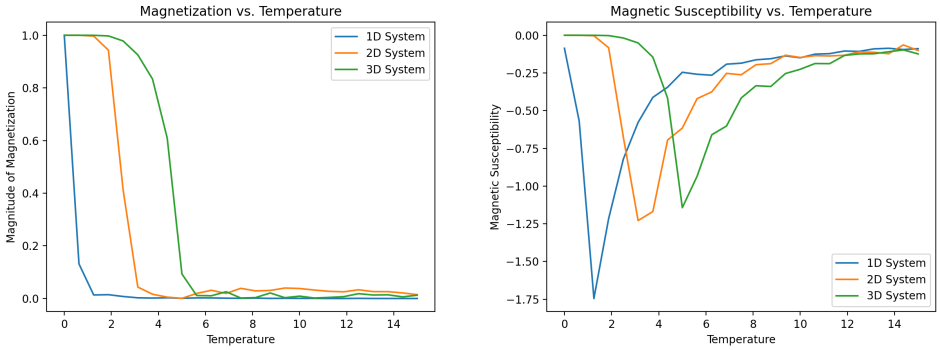

Figure 3.10
Magnetization (left) and susceptibility (right) plotted against temperature for case 3, with initial states of 90% up-spin.

Finally, the magnetization and susceptibility versus temperature for case 4 are given in Fig. 3.11. Results are shown for both 75% and 90% up-spin in the initial state.

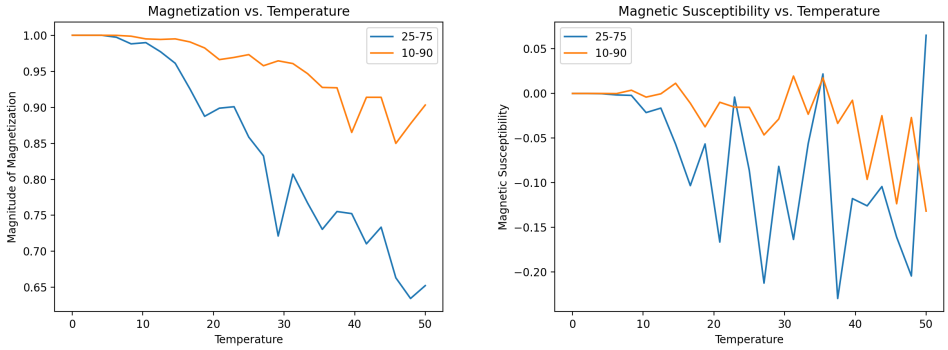

Figure 3.11
Magnetization (left) and susceptibility (right) plotted against temperature for case 4, with initial states of 75% and 90% up-spin.

3.3 Energy and Specific Heat vs. Temperature

The final set of tests first found the average energy of the system after reaching equilibrium using 1.5 while varying the temperature. The rate of change of these results then gave the specific heat, as according to 1.2.

The energy and specific heat for case 1 is shown in Fig. 3.12.

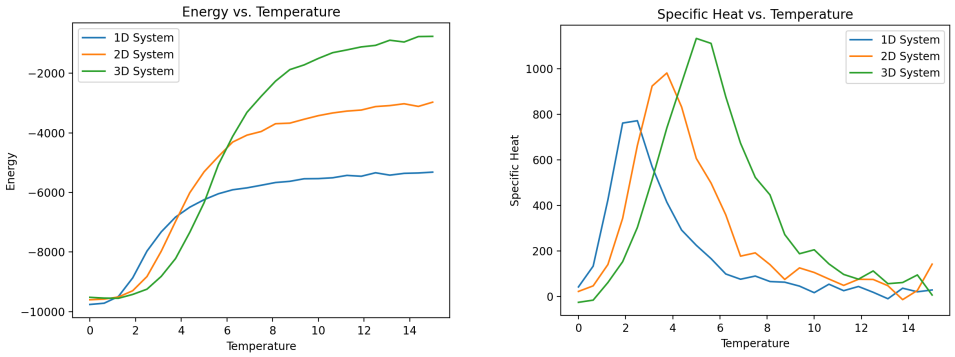

Figure 3.12
Energy (left) and specific heat (right) with respect to temperature for case 1

The energy and specific heat for case 2 is shown in Fig. 3.13.

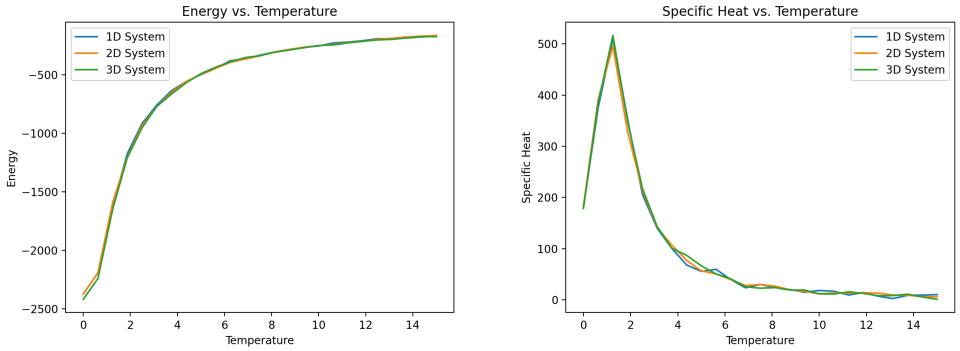

Figure 3.13
Energy (left) and specific heat (right) with respect to temperature for case 2

The energy and specific heat for case 3 is shown in Fig. 3.14. In this case, the initial state was weighted to be 90% up-spins, as previously established.

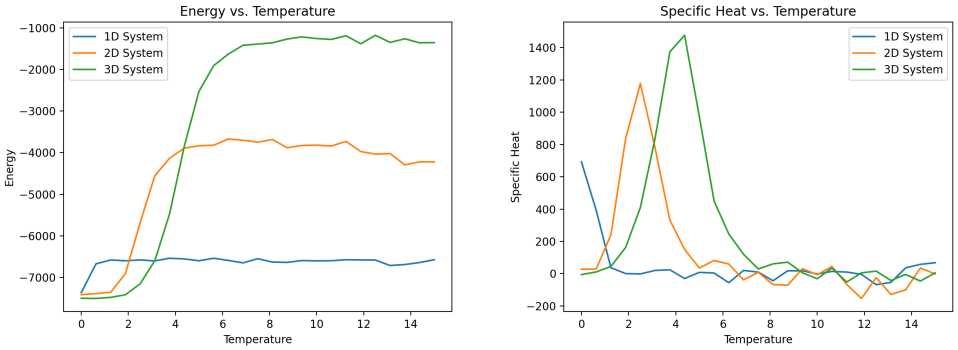

Figure 3.14
Energy (left) and specific heat (right) with respect to temperature for case 3 with 90% up-spins in the initial state

Finally, the energy and specific heat for case 4 is shown in Fig. 3.15. In this case, both 75% and 90% up-spins weightings are shown.

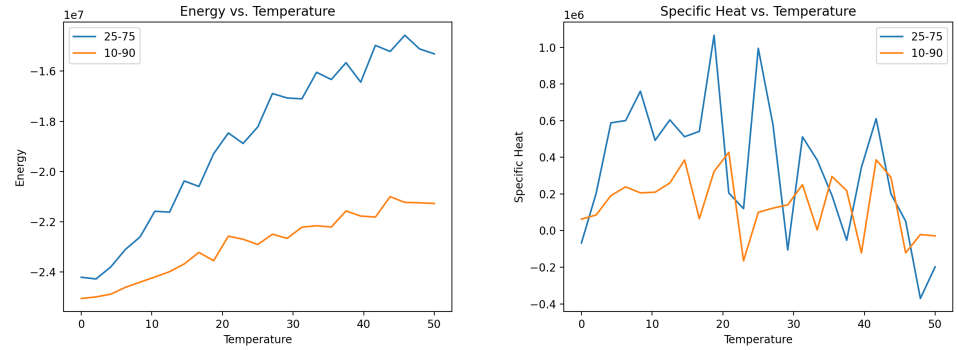

Figure 3.15
Energy (left) and specific heat (right) with respect to temperature for case 4 with 90% up-spins in the initial state

4 Analysis

Based on the results of magnetization over time for each test, cases 1 and 2 consistently reach equilibrium within 1-3 cycles (2500-7500 steps). In both cases, the magnetic field forces the spins into the down orientation, since μ is set to 1. Case 1 takes slightly longer than case 2, as it includes electrostatic interactions which make it more difficult to flip spins if their neighbors are aligned. This effect is more noticeable in higher dimensions, where there are more neighboring particles and thus stronger opposition to some intermediate states.

These electrostatic interactions are also the reason that, for significant enough up-spins, the equilibrium state is entirely up, rather than down (as it was with a mixed initial state). The three-dimensional case requires the smallest shift in the upward direction, since it has the most neighboring interactions, while the one-dimensional case appears to require far more than 90% of the initial spins to be up in order to assume a different equilibrium state.

When varying the temperature, the susceptibility and specific heat of both case 1 and case 2 seem to scale according to the total electrostatic interaction. Susceptibility inversely scales with this value, and specific heat directly scales with it.

$$\chi(\boldsymbol{S}) \propto \frac{1}{J_{total}} \tag{4.1}$$

$$C(\boldsymbol{S}) \propto J_{total} \tag{4.2}$$

This behavior matches known expectations, as increased electrostatic interactions decrease the overall effect of the magnetic field, while also increasing the amount of energy that can be stored.

There also seems to be a critical temperature at which the susceptibility and specific heat peak. This temperature seems to directly scale with the total electrostatic interaction.

$$T_c \propto J_{total} \tag{4.3}$$

This matches known expectations, which give us the following equation for critical temperature, where z is the number of interacting neighbors [1]:

$$T_c = \frac{zJ}{2k_B} \tag{4.4}$$

Above this temperature, magnetization drops off towards 0, at a rate proportional to the electrostatic interaction. Below this temperature, it approaches an equilibrium state determined by the overall field. For cases without electrostatic interactions, the behavior matches the results from Eq. 3.1. For cases with electrostatic interaction, the curve still matches the hyperbolic tangent, but due to the interactions is able to stay magnetized longer and thus has certain adjustments based on J:

$$\boldsymbol{M}_{\text{theoretical}} = \tanh\left(\frac{\mu B}{k_b T} + f(J)\right) \tag{4.5}$$

where $f(J)$ is some function of J.

As for the energies of cases 1 and 2, below the critical temperature they settle on similar values for all dimensions, with the interactions from case 1 greatly increasing the magnitude of this energy. Above the critical temperature they rapidly rise, with the rise slowing down as the temperature is further increased. This may imply a phase change, though since the energy does not entirely level out, it is also possible that there is no physical phase change.

As for cases 3 and 4, true equilibrium is only reached when the spins are significantly shifted in one direction. Without this shift, it takes on average 2-5 cycles to reach a random unstable equilibrium composed of various domains (for case 3, the domains have no specific pattern, but in case 4 the domains are oriented such that their x-dimension tends to be elongated). With a shift towards up-spin in the initial state, an equilibrium state of entirely up-spins is reached after 2-4 cycles. This behavior is inverted if the initial state instead favors down-spins.

When varying temperature, the susceptibility and specific heat of cases 3 and 4 have some important differences when compared to cases 1 and 2. In case 3, the peaks are much sharper and the critical temperatures are lower. In one dimension, the critical temperature appears to be 0, or at least very near 0. In case 4, due to incredibly strong electrostatic interactions, the peaks are extremely shallow and the critical temperature is very high.

These interesting behaviors are made more visible when viewing the magnetization and energy against temperature. In case 3, above the critical temperature the magnetization almost immediately drops to 0. Below the critical temperature, the magnetization levels off at the previously established equilibrium state. The energies show similar behavior, levelling off at a low value below the critical temperature and a high value above it. These results clearly show a phase change from aligned to randomly oriented, with the except of one dimension, which does not have a phase change. These results match known calculations about the Ising model.

For case 4, behavior is similar to case 3, but again with the critical temperature being much higher. In general, electrostatically interacting particles outside of a field give way to a phase change for dimensions of 2 or greater.

5 Discussion

The results of this report match known data about the Ising model. Behaviors of energy and magnetization (and their related values) match the established theoretical behaviors, specifically when it comes to phase changes and equilibrium states.

While the Metropolis-Hastings algorithm is highly suited to simulating smaller systems, as the system is scaled up it becomes increasingly slow. One way of remedying this is to run tests across multiple cores. States could be flipped in a checkerboard pattern (or similar) to prevent interference. Future iterations of the code should include this modification.

While the Ising model is fairly simple, it does have important applications to certain fields of science, especially for those studying behavior of metals or certain types of lattice-like materials. If this code is properly expanded, it can easily provide analytical results for almost any setup that is being studied.

REFERENCES

[1] Fitzpatrick, Richard (2006, March 29). *The Ising Model*.
http://farside.ph.utexas.edu/teaching/329/lectures/node110.html

[2] Wikipedia (2021, March 23). *Metropolis–Hastings algorithm*.
https://en.wikipedia.org/wiki/Metropolis%E2%80%93Hastings_algorithm