18.330 Final Project: A Numerical Model of Ising Ferromagnets

Justin Xiao

May 2017

1 Introduction

One of the earliest questions to arise in physics is: how do ferromagnets work? It became clear in the early twentieth century that classical physics would not be sufficient to explain the phenomenon, by the Bohr-van Leeuwen theorem. Physicists then turned to quantum mechanics to find the answer.

In quantum physics, electrons have a fundamental property of spin, which can only be in either state up or state down. With these spins come an associated magnetic moment, such that, when enough such moments are aligned, a noticeable magnetic field is created. In an atom with filled electron shells, Pauli's exclusion principle, which precludes fermions from sharing the same state, causes the total spins to cancel out and leaving a net zero dipole moment. However, in materials with partially filled shells, we see that the electrons start sharing the same spin alignment. In the presence of a magnetic field, these moments align and create a magnetic field, known as paramagnetism. In ferromagnets, however, the moments may spontaneously align, creating the magnets you see around you daily, whether on your fridge or in your speakers.

One of the simplest models for a ferromagnet is given by the Ising model, which is represented by a fixed lattice of spins, which either point up (+1) or down (-1). The problem of a one-dimensional lattice was solved by Ising in 1925, and it was shown that a one-dimensional lattice does not produce a phase transition, instead exhibiting spontaneous magnetization at any positive temperature. The problem of the two-dimensional square lattice Ising model was solved in 1944 by Lars Onsager, where he showed that indeed, such a system exhibits a phase transition from ferromagnetic to non-ferromagnetic above some critical temperature.

While the Ising model is a very good model of how ferromagnets behave, it is also theoretically and historically significant in that it was one of the first demonstrations of modelling phase transitions from statistical models, which lead to a much deeper understanding of both statistical mechanics and phase transitions.

Prior to the Ising model, there was high disbelief in the ability of statistical mechanics to model phase transitions. One argument is as follows. Since the partition function is exponential as a function of β, and thus analytic, and since the sum of analytic functions is also analytic, phase transitions cannot arise from the partition function. However, in the thermodynamic limit, there arises an infinite sum which leads to singularities, producing phase transitions. This occurs even for a finite lattice, which rapidly approaches the thermodynamic limit.

2 History of the Metropolis Algorithm

In order to solve the Ising model numerically, we use the Metropolis algorithm. This algorithm is an example of a Markov Chain Monte Carlo algorithm, used to generate samples from some probability distribution.

The history of Markov Chain Monte Carlo methods goes back to the 1940's at Los Alamos, where many noteable mathematicans and scientists were working on the Los Alamos project. It began with Stan Ulam, who, while playing solitaire, thought of the question of: given an initial configuration of cards, what is the probability of winning a game of solitaire? After tackling the problem with various combinatorics methods, he concluded that a computer could help solve the problem by simulating multiple configurations and finding how many times it wins for such configurations. Around the same time the first computer, the ENIAC, was developed and used in these computations.

This idea of using sampling and statistical methods with computers was adopted by John von Neumann, who used the idea in calculations with neutron diffusion. Nicholas Metropolis suggested the name "Monte Carlo" for the algorithm, based on the famed casino. After this initial implementation, the physics literature boomed with papers on Monte Carlo methods.

In 1953, Nicholas Metropolis introduced the first Markov Chain Monte

Carlo method. The purpose was to calculate integrals of the form

$$\frac{\int f(\theta)e^{-E(\theta)/k_BT}d\theta}{\int e^{-E(\theta)/k_BT}d\theta}$$

which is a standard computation in statistical physics, given that e^{-E/k_BT} represents the Boltzmann distribution, with k_B being the Boltzmann constant and parameterized by energy E and temperature T. θ represents a set of N particles on $\mathbb{R}^2$, and is thus a $2N$-dimensional array. This makes standard numerical integration intractable. Due to the smallness of the Boltzmann distribution for most configurations, standard Monte Carlo methods are similarly unable to solve the problem.

Metropolis' proposed solution goes as follows. For every particle i, vary its position by some amount uniformly distributed between $[-\epsilon, \epsilon]$. Calculate the change in energy ΔE for this variation, and accept the change with probability $min\left(1, e^{-E(\theta)/k_BT}\right)$. As applied to the Ising model, instead of varying the position of the particles, we instead flip the sign of the spin.

3 The Metropolis Algorithm

In this section we go into more depth on the Metropolis algorithm and its application to the Ising model.

The Metropolis algorithm is designed such that a Markov chain approaches a unique stationary distribution $\pi(x)$ such that $\pi(x) = P(x)$. Given a Markov chain with transition from x to x', we have the probability of transition given by $P(x'|x)$. In order to satisfy our above requirement, we have two conditions to meet:

- We require the existence of a stationary distribution π. It is sufficient to require detailed balance, which states that any process is reversible such that the probability of transitioning from $x \to x'$ is the same as transitioning from $x' \to x$. This can be written as:

  $$\pi(x)P(x'|x) = \pi(x')P(x|x')$$

  .

- We require uniqueness of the stationary distribution, which is guaranteed by ergodicity, such that any state is aperiodic and recurrent.

We now apply these requirements to the Ising model. We assume that, given N spin sites, we have a selection probability of $g(x'|x) = 1/N$. We derive from detailed balance the following:

$$\frac{P(x|x')}{P(x'|x)} = \frac{g(x|x')A(x|x')}{g(x'|x)A(x'|x)} = \frac{A(x')}{A(x)} = \frac{e^{-\beta E_{x'}}}{e^{-\beta E_x}} = e^{-\beta(E_{x'}-E_x)}$$

where β is given by $1/k_B T$ and $A(x'|x)$ is the acceptance probability of going from $x \to x'$. We thus have an acceptance probability of

$$min\left(1, e^{-\beta(E_{x'}-E_x)}\right)$$

The algorithm is detailed below:

1. With probability $1/N$, go to some spin spite i
2. Calculate the contribution to the energy from spin i
3. Flip the sign of the spin at i
4. Re-calculate the energy associated with i
5. if the new energy is less than the old energy, keep the flipped spin
6. if the new energy is greater, keep the new spin with probability

$$A(x'|x) = e^{-\beta(E_{x'}-E_x)}$$

7. Repeat

To calculate the energy, we use the Hamiltonian given by

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j - h \sum_j \sigma_j$$

where J is the interaction strength, h is the magnetic field strength, σ_j represents the spin at site j, and the sum over $< i, j >$ represents a sum over the i nearest neighbors.

4 The Ising Model

We now discuss the theory behind the Ising model, starting from the one-dimensional case and extending it to the two-dimensional case. To solve these problems, we employ the method of transfer matrices.

4.1 1D Ising Model

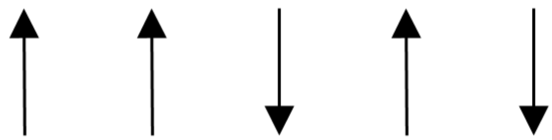

Figure 1: 1D Ising chain

In the one-dimensional Ising model, the Hamiltonian is given by

$$H = -J\sum_i \sigma_i\sigma_{i+1} - h\sum_i \sigma_i$$

Our partition function is then given by

$$\sum_{\sigma_1}\cdots\sum_{\sigma_N} e^{\beta\sum_{j=1}^{N}(J\sigma_j\sigma_{j+1}+\frac{h}{2}(\sigma_j+\sigma_{j+1})}$$

If we define the transfer matrix

$$P_{\sigma_i\sigma_j} = e^{\beta(J\sigma_i\sigma_j+\frac{h}{2}(\sigma_i+\sigma_j)}$$

then

$$P = \begin{bmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{bmatrix}$$

our partition function then becomes

$$Z = \sum_{\sigma_1} P^N_{\sigma_1\sigma_1} = Tr(P^N)$$

Now, P has eigenvalues given by

$$\lambda_+ = e^{\beta J}\left(\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta h}}\right)$$

$$\lambda_- = e^{\beta J}\left(\cosh(\beta h) - \sqrt{\sinh^2(\beta h) + e^{-4\beta h}}\right)$$

Now, since $Z = Tr(P^N) = \lambda_+^N + \lambda_-^N$, we find that our partition function is

$$Z = e^{N\beta J}\left(\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta h}}\right)^N$$
$$+e^{N\beta J}\left(\cosh(\beta h) - \sqrt{\sinh^2(\beta h) + e^{-4\beta h}}\right)^N$$

In the large N limit, λ_+ dominates, so our partition function is approximated as

$$Z = e^{N\beta J}\left(\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta h}}\right)^N$$

From the partition function, we can calculate any thermodynamic variable of interest. Particularly, we are interested in the internal energy U, magnetization M, specific heat C, and susceptibility χ.

We start by calculating the internal energy, which is given by $U = -\frac{\partial ln(Z)}{\partial \beta}$. To simplify further analysis, we set $h = 0$, such that we calculate the contribution to the energy from spin interaction alone. In this case, $Z = (2\cosh(\beta J))^N$, so we find that, for the 1D Ising chain, the internal energy is given by

$$U = -JN\tanh(\beta J)$$

Heat capacity is defined to be $\frac{\partial U}{\partial T}$, so we calculate

$$C_V = \frac{NJ^2\,\mathrm{sech}^2(\beta J)}{T^2}$$

These two quantities are plotted below.

For more interesting variables, we now analyze the magnetization M. To derive this quantity from the partition function, we use the equation $M = \frac{1}{\beta}\frac{\partial \ln(Z)}{\partial h}$ to get

$$M = \frac{N\sinh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}$$

The susceptibility is given by $\chi = \frac{1}{N}\frac{\partial M}{\partial h}$. Plugging in our expression for M, we get

$$\chi = \frac{\beta\cosh(\beta h)}{(1 + e^{-4\beta J}\sinh^2(\beta h))\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}$$

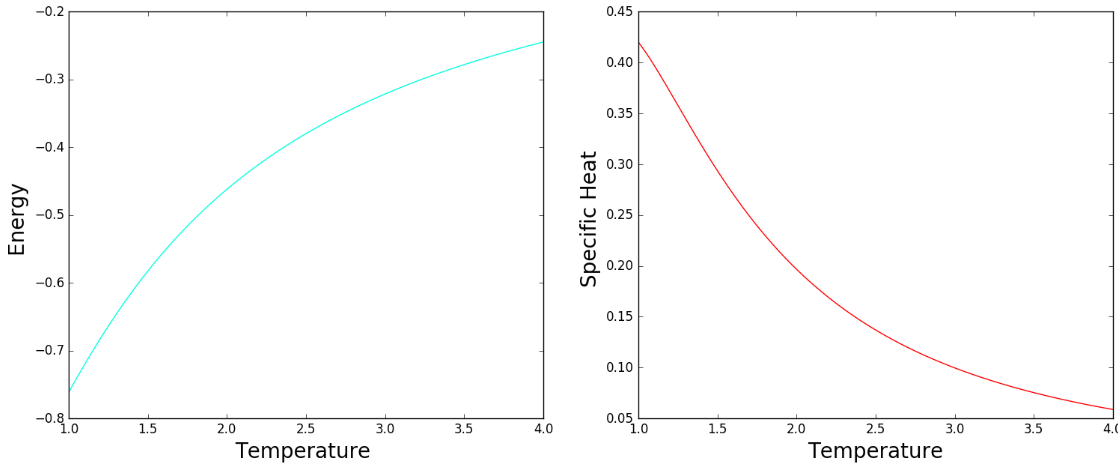

Figure 2: Energy and Specific Heat of 1D Ising chain

These two quantities are plotted below, for $h = 1$.

An interesting fact to note from this analysis is that spontaneous magnetization does not occur for any positive temperature. This implies that for the one-dimensional Ising model, there is no phase transition! Thus, the critical temperature for a 1D chain is $T_C = 0$.

4.2 2D Ising Model

We now analyze the 2D Ising square lattice, which has more interesting properties than in the one-dimensional case. However, we will not go into great mathematical depth, since the process is very involved. Instead, I will state the important results. Additionally, we will look only at the case of $h = 0$, since otherwise there is no as-of-yet solved for analytic solution.

The partition function is given by

$$Z = \sum_{\sigma} e^{\beta J \sum_{<i,j>} \sigma_i \sigma_j}$$

where we sum over all spin configurations and calculate contributions from nearest neighbors (not including diagonal neighbors).

By Kramers-Wannier duality, which maps an Ising model at low temperature to one at high temperature. Denote the interaction term for the low

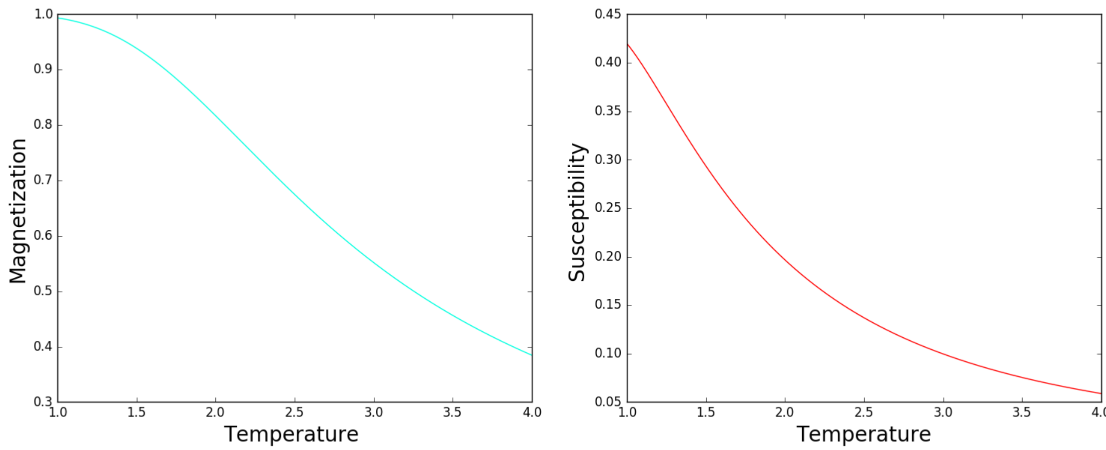

Figure 3: Magnetization and Susceptibility of 1D Ising chain

temperature Ising model as J^*, and for the high temperature Ising model as J. The low temperature partition function is then given by

$$Z(J^*) = 2e^{2\beta N J^*} \sum_P (e^{-2\beta J^*})^{r+s}$$

Using the transformation

$$\tanh(\beta J) = e^{-2\beta J^*}$$

we have

$$Z(J^*) = 2(\sinh(2\beta J))^{-N} Z(J)$$

Calculating the free energy using the Kramers-Wannier duality, we see that

$$f(J^*) = f(J) + T\ln(\sinh(\beta J))$$

This implies a critical temperature, at which $f(J^*) = f(J)$, such that

$$sinh(\beta J) = 1$$

and thus we have the well-known expression for T_C,

$$T_C = \frac{2J}{\ln(1+\sqrt{2})} \approx 2.7J$$

The internal energy is given by

$$U = -J\coth(2\beta J)\left[1 + \frac{2}{\pi}(2\tanh^2(2\beta J) - 1)\int_0^{\pi/2}\frac{1}{\sqrt{1 - 4k)(1+k)^{-2}\sin^2(\theta)}}d\theta\right]$$

where the last integral is related to the elliptic integral of the first kind, and $k = \frac{1}{\sinh 2\beta J}$.

The energy as a function of T, along with the heat capacity (which is too complicated to write here), are plotted below, with $J = 1$.

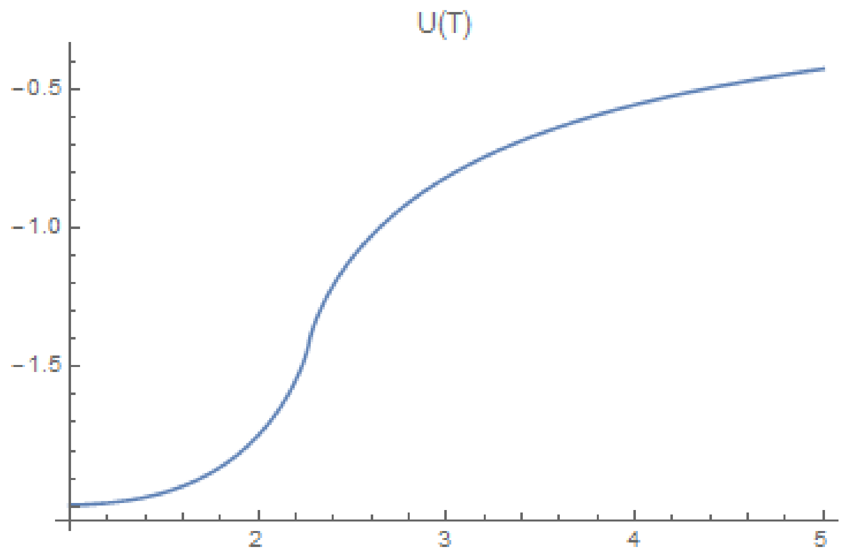

Figure 4: Internal Energy of 2D Ising Lattice

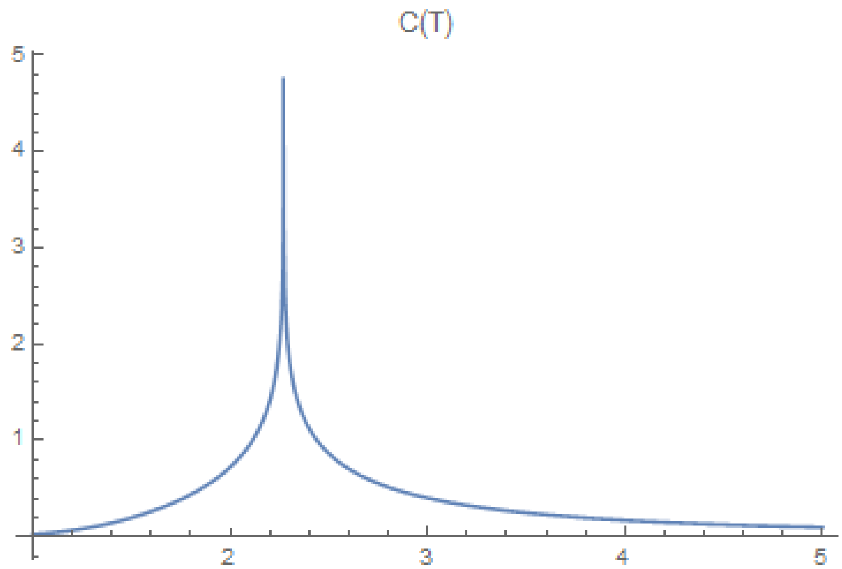

Figure 5: Heat Capacity of 2D Ising Lattice

We can see, by looking at the plot for heat capacity, where the critical temperature is. By looking at the temperature at which the sharp peak occurs, we determine that the critical temperature is indeed at 2.7.

We now look at the spontaneous magnetization of the 2D Ising lattice, which is given by

$$M(T) = \begin{cases} (1 - \sinh^{-4}(2\beta J))^{1/8}, & \text{if } T < T_C \\ 0, & \text{if } T > T_C \end{cases}$$

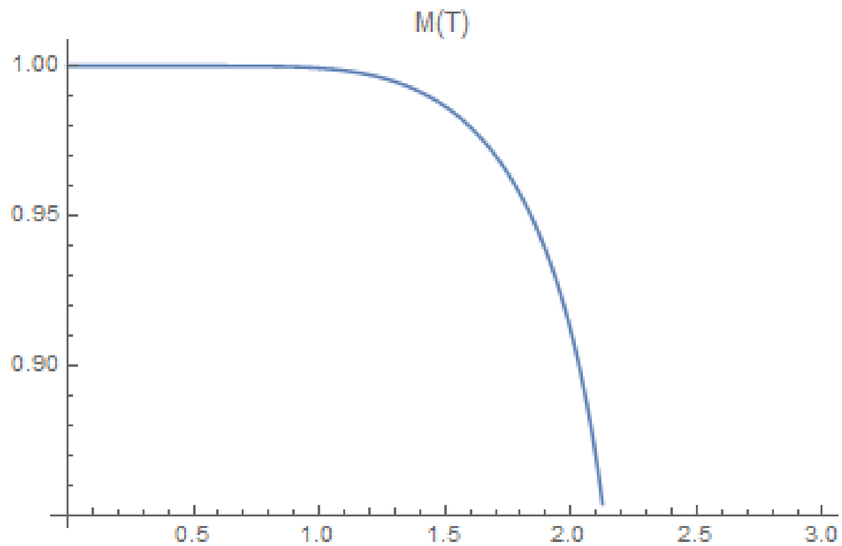

Figure 6: Spontaneous Magnetization of 2D Ising Lattice

We see that, for the spontaneous magnetization, as T approaches the critical temperature, dies to 0. The susceptibility, as far as I can tell, has no simple analytic form.

5 Numerical Results

In this section we now present results from numerical simulation.

The general algorithm for updating spins is the same as outlined in the section on the Metropolis algorithm. To calculate the thermodynamic variables of interest, we do the following:

- For any quantity at some temperature, we thermalize the states by updating 20000 times before averaging the measured quantity over 10000 calculations.
- Energy: We directly calculate the Hamiltonian, summing over nearest neighbors and calculating the contribution from external magnetic field at each spin. We then find the average energy over 10000 calculations.
- Magnetization: We can calculate the magnetization by summing over all spin sites. We average this quantity over 10000 calculations.

- Specific Heat: This can be calculated by averaging E^2 over 10000 calculations, and calculating

$$C_V = \frac{(\langle E^2 \rangle - \langle E \rangle^2)}{T^2}$$

- Susceptibility: Similar to the specific heart, we can calculate

$$\chi = \frac{(\langle M^2 \rangle - \langle M \rangle^2)}{T}$$

5.1 2D Ising Lattice Simulation

We now present our numerical results for the two-dimensional lattice. Our main results are shown in the figure below.

Using our results from our theoretical treatment, we see that we can pick out the critical temperature by looking at where the maximum occurs in the specific heat and susceptibility. In this case, it occurs at 2.30, which is very close to the theoretical value! Comparing the shapes of the plots to the theoretical case as well, we see very close matches. Thus, we see our numerical analysis is successful for the two-dimensional lattice.

We now visualize the lattice for various values of J, T and h. For $J = 1$ and $T = 1$ with $h = 0$, which is less than the critical temperature, we see that all the spins in the lattice are aligned and so spontaneous magnetization has occured.

For $J = 1$ and $T = 2.3$, we see that there starts to be some demagnetization. At $T = 5$, well above T_C, there is more or less complete demagnetization and randomization of spins.

However, with T still at $T = 5$, if we introduce a strong external magnetic field such as $h = 7$, the spins begin to align strongly.

One more interesting case is if $J < 0$. When we do this, the lattice becomes anti-ferromagnetic, such that the lattice alternates spins. We see that, at every site the spin alternates from its neighbors.

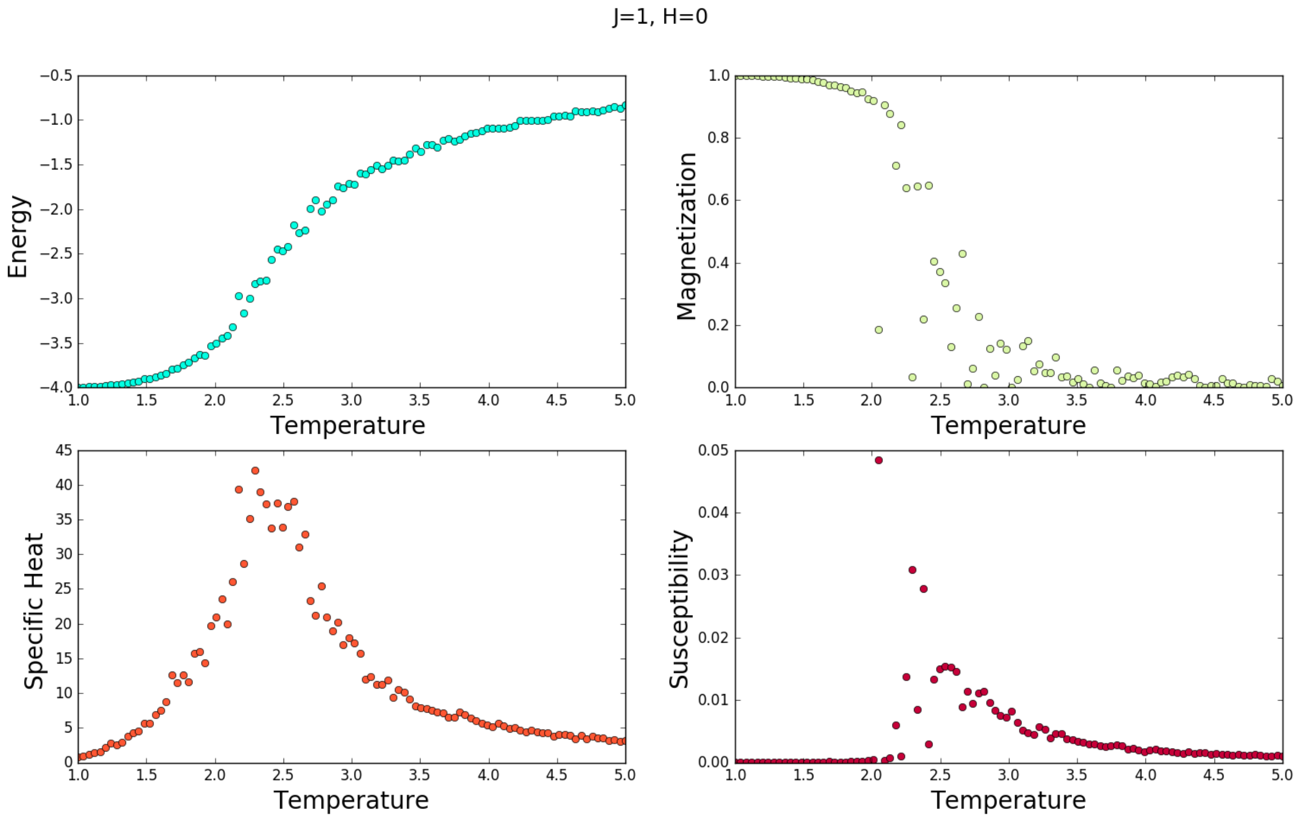

Figure 7: Simulation Results of 2D Ising Lattice

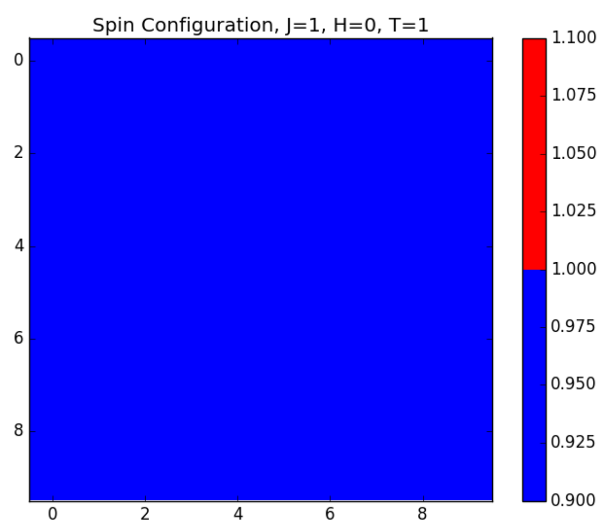

Figure 8: State simulation with $J = 1$, $T = 1$, which strongly exhibits spontaneous magnetization

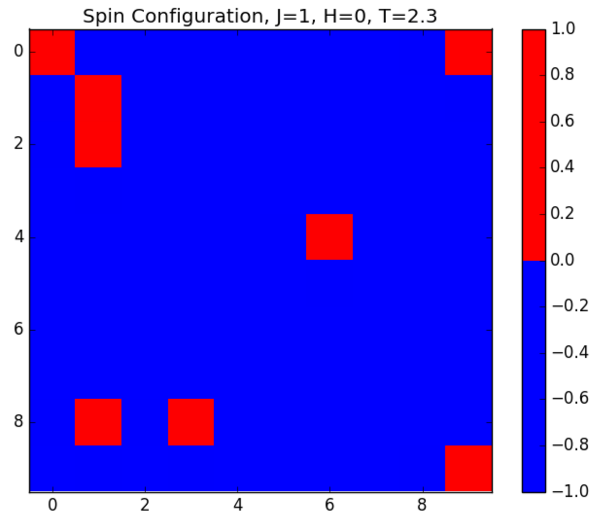

Figure 9: State simulation with $J = 1$, $T = 2.3$, which weakly exhibits spontaneous magnetization

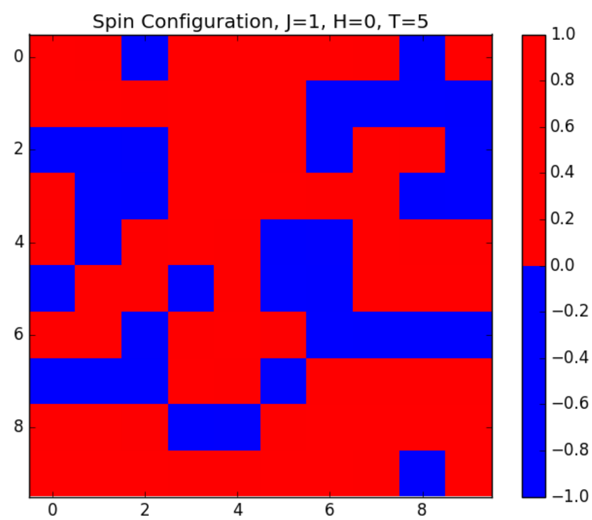

Figure 10: State simulation with $J = 1$, $T = 5$, which does not exhibit spontaneous magnetization

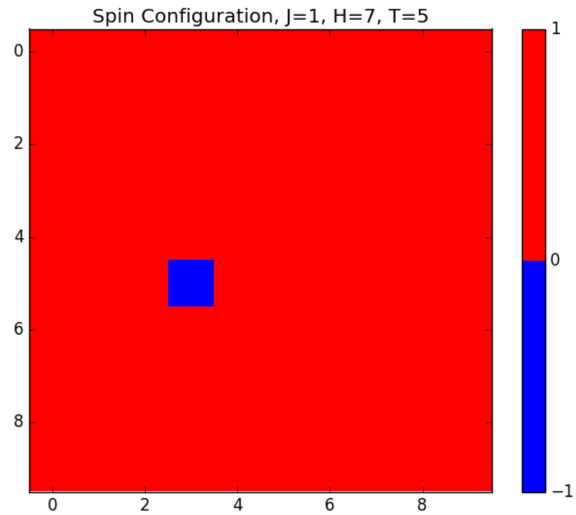

Figure 11: State simulation with $J = 1$, $T = 5$, and $h = 7$, with strongly aligned spins

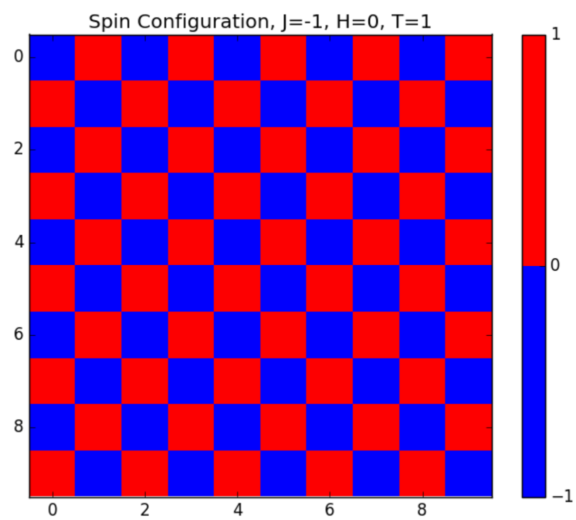

Figure 12: State simulation with $J = -1$ and $T = 1$, which strongly exhibits anti-ferromagnetism

5.2 3D Ising Lattice Simulation

While no simple analytic solution exists for the 3D Ising model, there are established results on the critical temperature, which is around $T_C \approx 4.45$. Looking at our plots for our simulation, we see that the maximum for the specific heat and susceptibility occur at $T_C = 4.1$, which matches decently well with the established result. Since the program takes a very long time to run (scaling as N^3), I had to use a small lattice size to run the program in reasonable time. By increasing the lattice size to better approach the thermodynamic limit, the measured critical temperature would be closer to the established value.

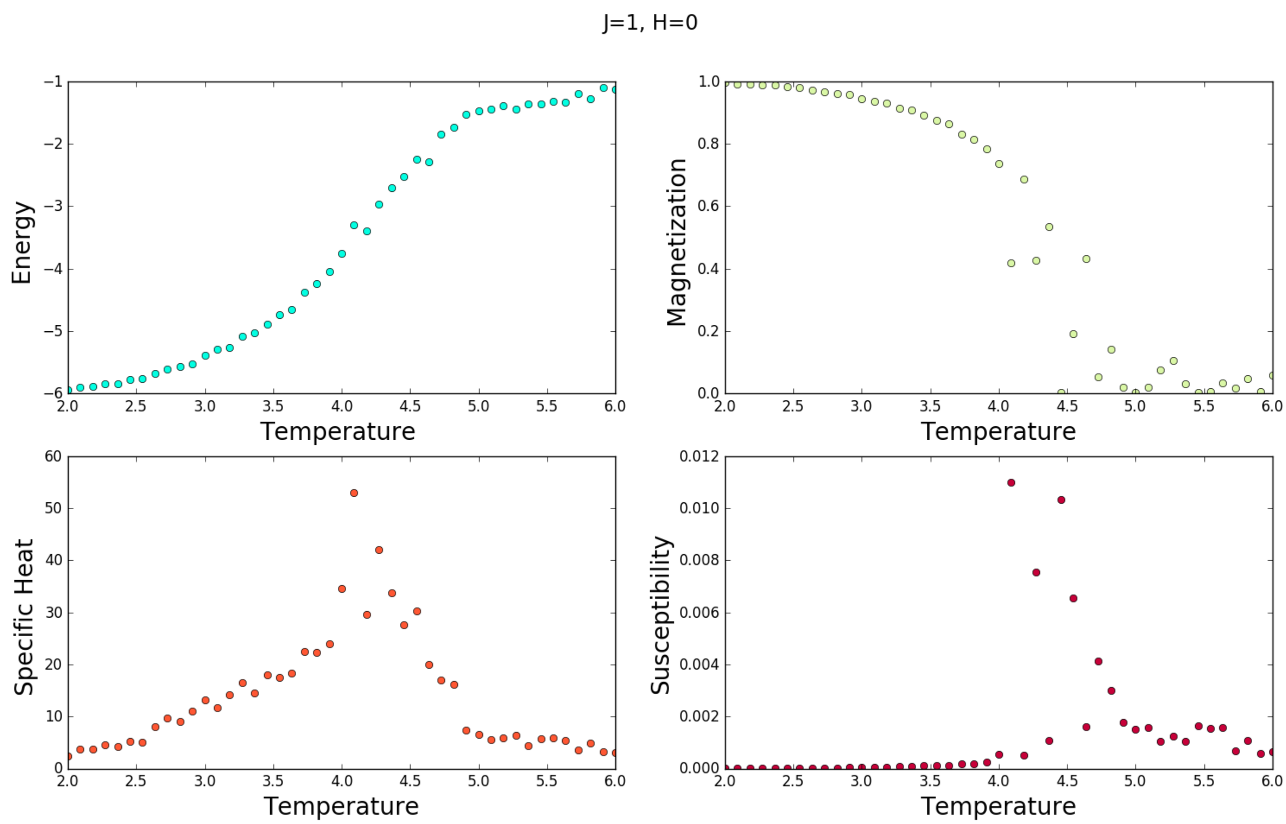

Figure 13: Simulation Results of 3D Ising Lattice