Computational Physics: The Ising Model

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Abstract

In this report, the 2-dimensional Ising system was studied using a Monte-Carlo simulation based on the Metropolis Algorithm. A system of 2500 spins in a square lattice was simulated at varying temperatures and magnetic fields to obtain the critical temperature. Furthermore, the magnetisation and energy per spin and specific heat and magnetic susceptibility were determined as function of temperature. Lastly, the effect of a magnetic field on the magnetisation of the system was studied.

1 Introduction

Monte Carlo experiments are a general group of computational methods that rely on random sampling of particularly complicated models to generate useful numerical results. They have broad applications across physics (fluid dynamics, stellar evolution, etc.) and are often a "last-resort" solution for modelling very complicated systems. In particular, these methods are useful in systems or models that can be described probabilistically, especially when such systems have many parameters whose values may be coupled in some way.

For this project, we used a Markov-Chain Monte Carlo (MCMC) method to study the physics of the Ising model. The three-dimensional Ising model has no exact analytical solution yet, so numerical simulations are a valuable resource. That being said, for the purposes of this project, we only analyse the two dimensional system. Ising model systems are useful in studies of magnetism, and are sufficiently complicated to warrant the use of a Monte Carlo method.

In the report, we'll first explain the theory behind the Ising model. In the next section our methods are discussed. In particular, we discuss the Monte Carlo integration, Metropolis algorithm and the initialisation of our simulations. Lastly, we present our results and discussion of these results.

2 Theory

2.1 Ising Model

The Ising model is a simple model to study magnetism. The model consists of a system of spins that can point either up or down. Between two neighboring spins, there is an interaction energy and the spins also gain magnetic energy in the presence of a magnetic field. The system is described by the following Hamiltonian:

$$H = -J \sum_{<i,j>} s_i s_j - H \sum_i s_i \tag{1}$$

where J is the interaction energy between two neighboring spins (s_i and s_j) and H is the magnetic field. As the spins can only point up or down: $s_i \in \{-1, 1\}$.

If the value of the interaction energy is positive ($J > 0$), the system will become ferromagnetic and all the spins will align at low temperatures. For a random starting configuration, both directions in which the spins can align (up or down) are equally likely in the absence of a magnetic field. If there is a magnetic field, the spins will align with the direction magnetic field. [Cipra 1987]

In both cases the Ising model has a phase transition for two dimensions or higher. At the critical temperature the system will go from an ordered, ferromagnetic system to a disordered system with zero magnetisation. The exact critical temperature is:

$$\frac{k_B T_c}{J} = \frac{2}{\ln 1 + \sqrt{2}} \approx 2.269 \tag{2}$$

in which T_c is the critical temperature.

Several interesting variables can be determined for the Ising model. The first one is the average magnetisation per spin:

$$m = \frac{1}{N^2} \sum_i s_i \tag{3}$$

where m is the magnetisation, N is the number of spins and s_i is the value of the spin.

Similarly, the average energy per spin can be obtained from the Hamiltonian (equation 1). The average total magnetisation and energy can be used to calculate the magnetic susceptibility (equation 4) and the specific heat (equation 5).

$$\chi_M = \frac{\beta}{N^2} \left(\langle M^2 \rangle - \langle M \rangle^2 \right) \tag{4}$$

where χ_M is the magnetic susceptibility, β is the inverse temperature, and M the total magnetization. The brackets indicate time averages.

The specific heat is given by

$$C_v = \frac{1}{N^2 k_B T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \tag{5}$$

where C_v is the specific heat, T is the temperature and E is the total energy of the system. [Swendsen 2012]

3 Methods

3.1 Monte Carlo Integration

To tackle the Ising model simulation, we use a Monte Carlo method known as Monte Carlo Integration. This method is of use in this context, because we are ultimately studying the statistical mechanics of this system, which will necessarily require calculating high-dimensional integrals. In quick terms, Monte Carlo integration for an integral $\int_a^b f(x)dx$ works to calculate the expectation value of f for a given probability distribution $p(x)$. This is done by by summing over f for a number, N, of states, x_i, that are randomly sampled according to $p(x)$. In the case of a uniform probability distribution, $p(x) = 1/(b-a)$, this looks as follows:

$$\begin{aligned} \int_a^b f(x)dx &= (b-a) \int_a^b \frac{1}{b-a} f(x)dx \\ &= (b-a) \int_a^b p(x) f(x)dx \\ &\approx \frac{b-a}{N} \sum_{i=1}^{N} f(x_i) \end{aligned} \tag{6}$$

This is preferable to "simpler" numerical integration methods (such as the rectangle method), because the error in the estimate does not scale with the system dimension. For MC integration, the error scales as $1/\sqrt{N}$ only, while the rectangle method (and other similar methods) error scales like $1/N^{k/d}$, where d is the system dimension, making the Monte Carlo integration superior for systems with many degrees of freedom.

Of course, in the case of statistical mechanics, the integrals we are looking to solve look more like

$$\int A(x) e^{-\beta H(x)} dx. \tag{7}$$

Where $\beta = 1/k_B T$ and H is the Hamiltonian of the system. The function $A(x)e^{-\beta H(x)}$ is very sharply peaked, making sampling over a uniform distribution very inefficient. Instead, we define the probability distribution to be $p(x) \propto e^{-\beta H(x)}$, and solve similarly.

$$\int A(x)p(x)dx \approx \frac{1}{N}\sum_{i=1}^{N} A\left(x_i\right) \tag{8}$$

Computationally, to ensure we are selecting with a similar probability distribution, we implement our Monte Carlo integration using a Metropolis Algorithm.

3.1.1 Metropolis Algorithm

The Metropolis Algorithm works by using a Markov Chain of different possible system states $\{x_i\}$, where the probability of a new state x' depends only on the current state x. The probability of each state in the chain existing at a step number i can be calculated with:

$$p(x, i+1) = p(x, i) - \sum_{x'} p(x, i)T\left(x \to x'\right) + \sum_{x'} p\left(x', i\right) T\left(x' \to x\right) \tag{9}$$

where $T\left(x \to x'\right)$ is the probability of transitioning from x to a given possible next state x'. In the case of our simulation, we want to look at the system when it is in thermal equilibrium. In this case, the probability distribution for a given state x should be stationary, so $p(x, i+1) = p(x, i)$. In this case, the above equation becomes:

$$\sum_{x'} p(x, i)T\left(x \to x'\right) = \sum_{x'} p\left(x', i\right) T\left(x' \to x\right). \tag{10}$$

For simplicity's sake, we require detailed balance:

$$p(x, i)T\left(x \to x'\right) = p\left(x', i\right) T\left(x' \to x\right) \tag{11}$$

The probability of transition, T, is dependent on two factors:

$$T\left(x \to x'\right) = w_{xx'} \times A_{xx'} \tag{12}$$

$w_{xx'}$ is the probability that x' is (or can be) the next proposed state. It is necessary that this value is symmetric, such that $w_{xx'} = w_{x'x}$. In our case, to simplify our Ising model, we choose to enforce that no two spins can flip simultaneously, so each new possible system state is simply the current state with a single spin flip. This means there are $N \times N$ "valid" next states, each with equal probability.

$$\omega_{xx'} = \begin{cases} 1/N^2 & x \text{ and } x' \text{ have one spin difference} \\ 0 & \text{otherwise} \end{cases} \tag{13}$$

In our code, this is implicitly implemented in two ways. First, by randomly selecting (from a uniform distribution) the (i,j) coordinates of the single spin to be flipped for the next possible state. Secondly, we make sure that for each time step taken, N^2 new possible states are tested by the chain, representing one full "sweep" of the array and flipping every spin once, on average.

$A_{xx'}$ is the probability that the x' is "accepted" as the new state, based on x. To satisfy equation 11, we can define the acceptance probability as:

$$A_{xx'} = \begin{cases} 1 & \text{if } p(x') > p(x) \\ p(x')/p(x) & \text{if } p(x') < p(x) \end{cases} \tag{14}$$

There is an additional physical interpretation of this result. In the context of statistical physics, we know that $p(x) \propto e^{-\beta H(x)}$ where H is the system Hamiltonian. This means that, for a given temperature, we can instead compare the energies of the systems to find A:

$$A_{xx'} = \begin{cases} 1 & \text{if } H(x') < H(x) \\ e^{-\beta \Delta E} & \text{if } H(x') > H(x) \end{cases} \tag{15}$$

Meaning, if the new proposed state's energy is less than the current state's, the transition will occur. If it's greater, the transition may occur depending on how large the increase is and the temperature of the system. At higher T, the probability of transition goes up. This perfectly fits our physical intuition: systems generally tend toward low-energy states, but high temperatures can prevent them from doing so. This is also important in terms of our code implementation. For one, calculating ΔE is easier than comparing the full probabilities. Also using ΔE instead of the individual Hamiltonians saves memory and prevents overflow when calculating A.

With this, one time step of the Metropolis Algorithm for our Ising model works as follows:

1. Create an initial system array of $N \times N$ spins to be the current state x. Calculate and save its energy. (See section 3.1.2 for a further explanation of how we deal with initial conditions.)
2. Randomly select a spin to flip. The next state, x', is simply x, but with this one spin pointing in the opposite direction.
3. Calculate the energy of the proposed state, compare the energies of x and x' and calculate A according to equation 15. Accept or reject the move from x to x' with respective probabilities A and 1-A. If accepted, set $x = x'$

4. Repeat steps 2 and 3 a total of N^2 times, representing one "sweep" of the system array.

This is done for as many time steps as the user inputs into the code.

3.1.2 Initial Conditions

When we analyse our Ising model, we want to make sure we do so only after the system has reached a state of thermal equilibrium. In practice, we have to wait until the average magnetisation per spin (AMS) in the model has reached a generally constant value. However, we can also use our physical intuition (confirmed with testing) to establish our initial conditions such that the model begins in thermal equilibrium. We know that the Ising model has a certain critical temperature (T_c) at which the behaviour at thermal equilibrium changes. Below this critical temperature, the model will tend toward a state where all the spins point in the same direction ($AMS = 1, -1$). Above this temperature, the model will tend to a random state where $AMS \approx 0$. We also know from theory (Alexandrou et al. 2020) that for a 2D, infinite-lattice Ising model, $T_c \approx 2.269$. This means that, in principle, if we start the models with $T < T_c$ at all up or all down, and the models with $T > T_c$ with randomly distributed initial values, they will begin in a state of thermal equilibrium, and our analysis can be conducted from the start.

To test this, we repeatedly run the Ising models at various temperatures with random initial conditions. In doing so, we can see that the AMS of the models at temperatures below T_c generally go to 1 or -1 (see figure 1). There are a few cases where the low-temperature models don't quickly flip to all up or all down, but these cases can be explained with the way the Markov Chain steps through states. It is expected that an unlucky "draw" of initial conditions would exhibit this behaviour, especially at temperatures near T_c. This actually becomes further evidence to support forcing the initial conditions of the system to be at thermal equilibrium, as it will sometimes take so long to reach that point, it becomes a waste of time, energy, and computing power.

We can repeat this test by starting all the models in either an up or down position, and we see the opposite behaviour: all the low-temperature models remain in roughly the same AMS, while the high-temperature models tend toward 0 AMS (see figure 2).

After completing these tests, we added a variable T_crit into the code. This represents the expected critical temperature, and defaults to 2.269. For the input models, if the model temperature is less than this value, the array is initialised to all being ± 1, if it is more than this value, each spin randomly takes a value of ± 1 according to a uniform distribution.

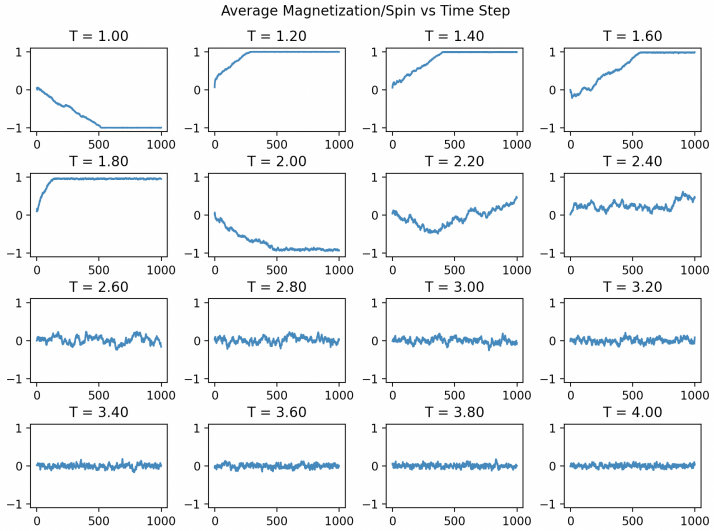

Figure 1: An example run to justify pre-setting the initial conditions to thermal equilibrium.

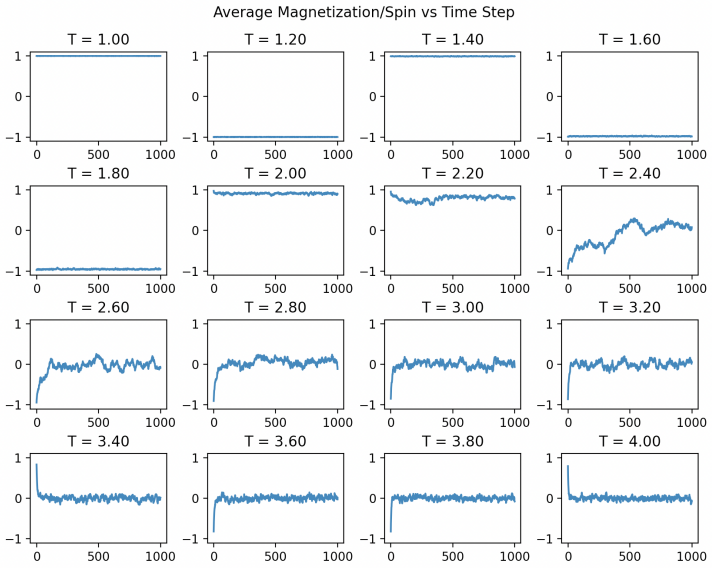

Figure 2: An example run to test initial conditions, this time starting all the models in a state of all up or all down.

4 Results

The following figures show the results of a simulation of 2500 spins in a square lattice in the absence of a magnetic field.

Figure 3 shows the correlation times for the different temperatures. The graph shows a clear peak around a temperature of 2.4 J/k_B.

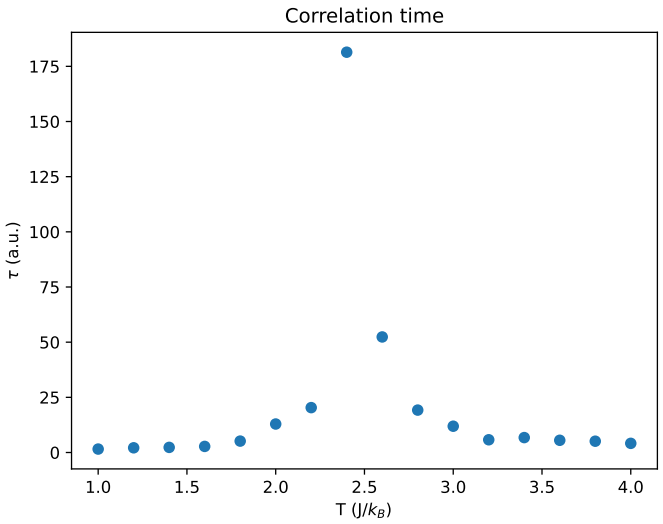

Figure 3: The correlation time (in arbitrary units) as function of temperature (in units of J/k_B where J is the interaction energy. The correlation time peaks around T = 2.4 J/k_B.

The average magnetization per spin is shown in figure 4. Here, the absolute value of the magnetization was taken, as there is no preferred direction for the spins to align with. The values -1 and 1 are thus equivalent. The figure shows that the magnetization is 1 for low temperatures. After T = 2.2, the magnetization drops rapidly to 0 as expected.

In figure 5 the average energy per spin is shown. For low temperatures, the energy is -2.0 which corresponds to the state in which all spins are aligned with each other. For high temperatures, the energy goes to -0.6. This is expected for a random state: some spins will still be aligned, which explains the non-zero value of the energy.

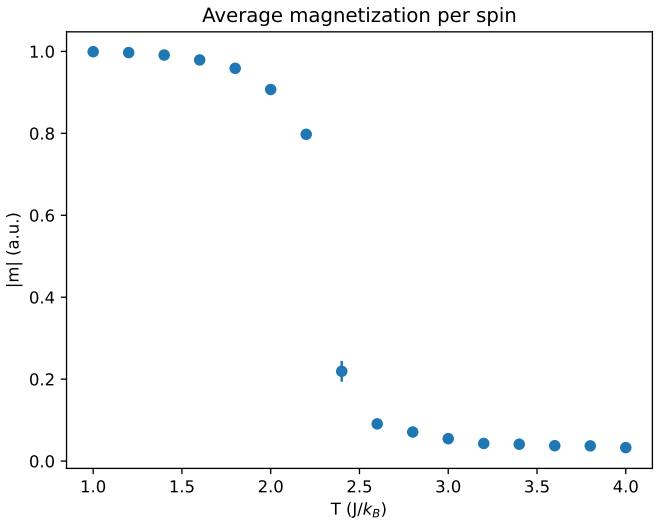

Figure 4: The average magnetization per spin (in arbitrary units) as function of temperature. For low temperatures, the (absolute) magnetization is close to 1, until the critical point when it goes to 0.

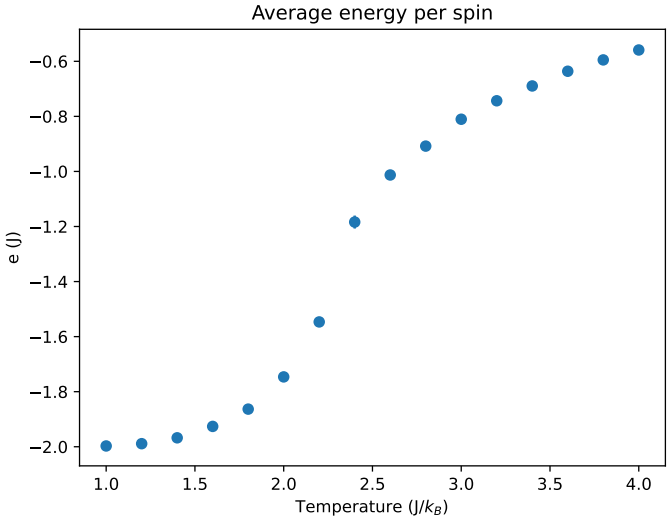

Figure 5: The average energy per spin (in units of J, the interaction energy) as function of temperatures. For low temperatures, the energy is -2.0, while for high temperatures the energy goes to approximately -0.6.

Figure 6 shows the magnetic susceptibility as function of temperature. The magnetic susceptibility also shows a peak at T = 2.4 J/k_B. However, there is a very large error for this data point. This is likely due to the fact that the correlation time becomes very large for this temperature. As a result, there are few data points to average over for this temperature, causing large fluctuations and thus a large standard deviation.

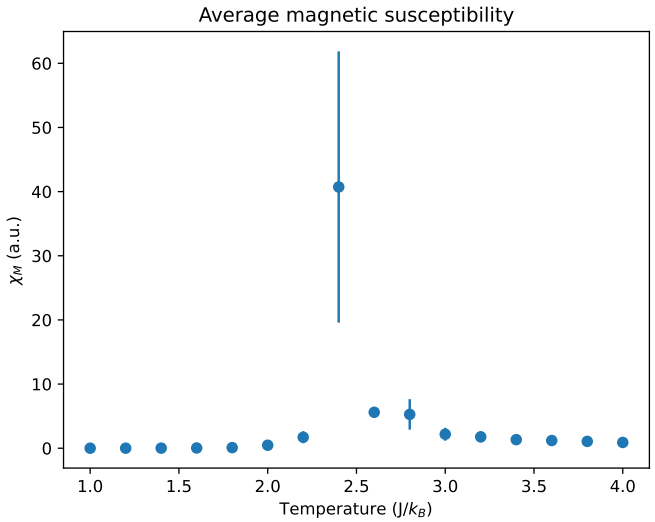

Figure 6: The average magnetic susceptibility as function of temperature. The graph shows a peak at T = 2.4 J/k_B.

Lastly, figure 7 shows the specific heat. This graph shows a peak at T = 2.4 as well. Similar as to figure 6, this data point has a very large error as well. This is most likely due to the same reason.

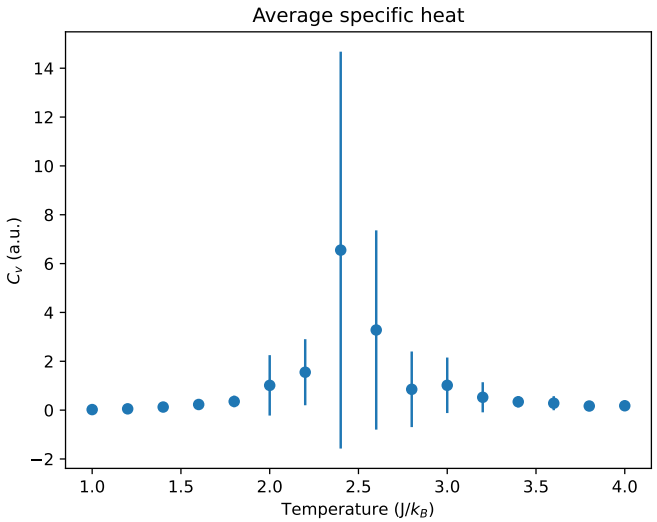

Figure 7: The average specific heat as function of temperature. The specific heat peaks around T = 2.4 J/k_B.

From the previous figures can be concluded that the critical temperature lies between T = 2.2 and T = 2.4 J/k_B, which is close to the theoretical value of T = 2.269.

4.1 Influence of a magnetic field

Figure 8 shows the magnetisation of the spin system for various magnetic field strengths. Clearly visible is that at high magnetic field strengths, the spins align with the direction of the field, regardless of the temperature of the system, as expected. Around H = 0, the direction of the field and thus the sign of the magnetisation changes. For temperatures below the critical temperature, this change is more sudden than for temperatures above the critical temperature.

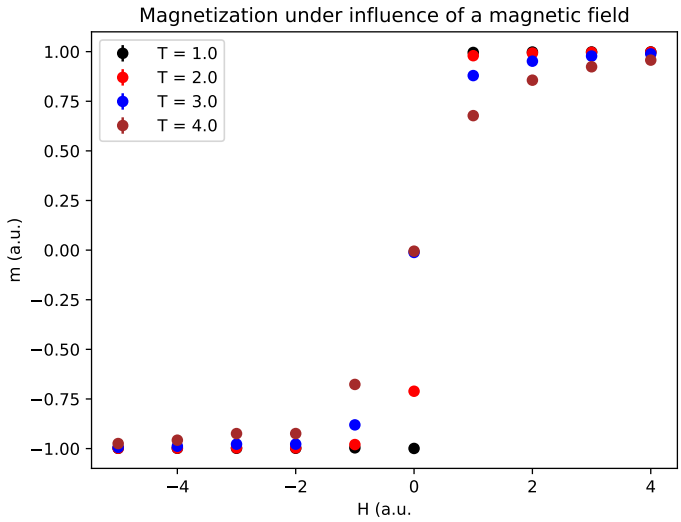

Figure 8: The magnetisation per spin (m) plotted against the magnetic field strength (H) for various temperatures. The curves for temperatures below the critical temperature (as found in the previous section) show a much steeper transition at H = 0 than the curves for temperatures above the critical temperature.

5 Conclusion and discussion

We have successfully simulated a 2D Ising model system with periodic boundary conditions. Our results reflect what we would otherwise expect from such a system, and indications of the critical temperature are in line with what is found in the literature ($T_c \approx 2.269$).

First, our magnetisation correlation time (figure 3) peaks between 2.2 and 2.6. The peak is sharp and distinct. We know that near the critical temperature, the average magnetisation per spin is more chaotic. As such, we expect the system to take a longer time to become uncorrelated at these temperatures.

For our average magnetisation per spin, average energy per spin, magnetic susceptibility, and specific heat, we can compare our plots to those found in figure 4.1 of Cosme 2014. Note that in Cosme 2014, these values are plotted with β on the x-axis, not temperature, so the plots are flipped compared to ours. That being said, the comparison can still be made. We can see in both our results (figure 4) and Cosme 2014 that for low T (high β), the absolute average magnetisation per spin is near 1, while for high T, it drops down to zero. We can also see that the drop is very abrupt, occurring around the expected critical temperature.

For the average energy per spin (figure 5), we see the energy starts out low for low T and increases with T. Generally, this pattern makes sense: in statistical mechanics, we obviously expect higher temperature systems to have greater average energy. The increase in average energy is not linear, with the change in energy per spin spiking around the critical temperature. The same can be seen in Cosme 2014.

The magnetic susceptibility (figure 6) and specific heat (figure 7) show similar patterns with fairly small, uniform values far from T_c, with a large spike at and around T_c. This is again in line with what we find in Cosme 2014. Additionally, looking at the plot of average energy per spin (figure 5) confirms for us that this should be what we expect for the specific heat. Specific heat is a measure of how much the energy of the system must be increased to reflect an increase in temperature. In figure 5, we see that around the critical temperature, the change in energy for a given change in temperature is visibly larger. This should (and does) indicate a higher specific heat for a system at this temperature.

While our results agree with previous research, one notable flaw is the large errors for the magnetic susceptibility and heat capacity near the critical point. As mentioned, this is most likely due to the fact that the correlation time is too long compared to our simulation time. Therefore, a useful next step would be to make our algorithm more efficient such that simulations with more time steps without taking too much time.

Finally, we look at the influence of a magnetic field on this system. In doing so, we compare the magnetisation per spin versus a number of magnetic field strengths (figure 8) for a number of temperatures. We can see from our plot that at all temperatures, the system generally aligns in the direction of the magnetic field. For small temperatures, this alignment is strong at even small values of H. For higher temperatures, relatively low (± 1) values of H do not induce as strong an alignment. This is generally expected, as in the H=0 case, where high temperature ($T > T_c$) systems did not align in either direction. That being said, the influence of the magnetic field generally causes the system (even at higher T) to align. This can be interpreted as an effective increase in critical temperature, where the critical temperature is known as the temperature at which the system goes from being aligned at thermal equilibrium to being random at thermal equilibrium. Similar results can be found found in figure 1a of Singh 2015.

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