PHSX815_Project4:
2D Ising Model Simulations

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1 Introduction

One of the key ideas in statistical physics is that atom-level interactions, over a large scale, lead to macroscopic properties of materials. Phase transition refers to a sudden change in the macroscopic properties of a material with varying temperatures. The temperature at which the phase transition occurs is called the Curie Temperature. The goal of this project is to study how spin interactions between atoms in a material cause phase transitions with sudden changes in energy, absolute magnetism, heat capacity, and susceptibility per spin in response to temperature changes.

To model the material and spin interactions, the 2D Ising Model is used in which the material is modeled as a 2D lattice, and spin interactions are modeled via coupling (1). The physical properties (energy, absolute magnetism, heat capacity, and susceptibility per spin) are numerically calculated. Since the 2D Ising Model can exhibit a phase transition (at least if there is no external magnetic field) (2), the physical properties calculated are analyzed for sudden changes near the Curie Temperature, which is also estimated theoretically.

The paper is divided into the following sections. Section 2 provides background knowledge on Ising Model. Section 3 discusses the pseudo code and the algorithm used to simulate Ising Model. Section 4 provides the results of the Ising Model simulation and provides numerical calculations of physical properties for varying temperature ranges. Next, best-fit models are generated to study the variation of these physical properties with temperature. An additional goal of this project is to study how well these best-fit models can actually model the relationship between these physical properties and temperature.

2 Background: Ising Model

Ising models refer to a general class of models that are used to study the physical properties of a material (1). In the 2D Ising Model, a material is modeled to be made up of atoms at lattice points that are fixed in space. Additionally, the atom at a lattice point (or simply, the lattice point) has a spin associated with it - either up (+1) or down (-1).
In this project, it is assumed that each lattice point can interact with just its immediate neighbor and there is no external magnetic field. The matrix below shows a 2D spin configuration composed of $n \times n$ lattice points, with random spins.

$$L = \begin{bmatrix} s_{1,1} & s_{1,2} & s_{1,3} & \cdots & s_{1,n} \\ s_{2,1} & s_{2,2} & s_{2,3} & \cdots & s_{2,n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ s_{n,1} & s_{n,2} & s_{n,3} & \cdots & s_{n,n} \end{bmatrix} \tag{1}$$

Here, $s_{i,j}$ refers to the spin of the atom at row i and column j. Each point (i, j), interacts with its four immediate neighbours $N(i, j) = \{(i-1, j), (i+1, j), (i, j-1), (i, j+1)\}$. It is worth noting that periodic boundary conditions are used. Hence, points at the edge interact with the "opposite" points. We define energy of a single lattice point $H(m)$ at $m = (i, j)$ as:

$$H(m) = -J \sum_{p \in N(i,j)} s_{i,j} s_p \tag{2}$$

Here, J determines the strength and the nature of interactions between neighboring lattice points. Considering that a system tries to minimize the energy, if $J > 0$, then each point favors the same spin as the neighbors. On the other hand, $J < 0$, then each point favors the opposite spin as the neighbor. Materials that favor the same spin alignment are called ferromagnetic materials, and exhibit absolute magnetism. On the other hand, materials that favor opposite sign alignment are called anti-ferromagnetic materials and don't exhibit absolute magnetism. In this project, J is set to 1.

Energy of the configuration: Assuming that there is no external magnetic field, the energy for a spin configuration L (denoted as $E(L)$) can be represented as

$$E(L) = \frac{1}{2} \sum_{m \in L} H(m) \tag{3}$$

Here, the summation is divided by 2 in order to not count the same spin twice in energy calculation.

Magnetism of the configuration: The magnetization of the spin configuration L (denoted as $(M(L))$) is defined as the "number of lattice points with spin up" - "number of lattice points with spin down". Since spin up and spin down are conveniently defined as $+1$ and -1, $M(L)$ is simply

$$M(L) = \sum_{(i,j)} L(i, j) \tag{4}$$

Probability of the configuration: The probability of a spin configuration L can be represented as

$$P(L) = exp(-\frac{E(L)}{kT}) \tag{5}$$

In this project, k is set to 1. Recall that J is also set to 1. According to the exact solution to Ising Model (2),

$$\text{Curie Temperature } T_c = 2.27 \frac{J}{k} = 2.27 \tag{6}$$

Calculating Observables: To calculate the average energy per spin, average absolute magnetism per spin, average heat capacity per spin, and average susceptibility per spin, a general model of computing an observable is constructed. The derivation below has been strongly inspired by (3).
Let $A(L)$ be observable that depends on the configuration L of the lattice. Here, observable refers to a physical property of the lattice that can be measured. For example, $E(L)$ (energy of the configuration) is an observable. The expected value of $A(L)$ (defined as $\langle A(L) \rangle$) is given as following:

$$\langle A(L) \rangle = \int A(L) P(L) dL \tag{7}$$

Setting $\beta = \frac{1}{kT}$ in equation (5),

$$\langle A(L) \rangle = \frac{1}{Z} \int e^{-\beta E(L)} A(L) dL \tag{8}$$

Here, Z is the partition function and defined as $Z = \int e^{-\beta E(L)} dL$. Approximating equation (8) with summations instead of integrals,

$$\langle A(L) \rangle = \frac{\sum_{i=1}^{N} e^{-\beta E(L_i)} A(L_i)}{\sum_{i=1}^{N} e^{-\beta E(L_i)}} \tag{9}$$

Here, L_i are the sample points drawn to evaluate $A(L_i)$. As $N \to \infty$, the absolute error between estimates of $\langle A(L) \rangle$ from (8) and (9) decreases. Notice here that L_i are unique, and that each L_i is evaluated individually, without replacement. That is, we evaluate the function $A(L_i)$ at L_1, then at L_2, then at L_3, and so on until we reach the last L_N.
The above equation (9) can be written as a stochastic process in which L_i are themselves drawn out of a probability distribution $F(L_i)$. Here, L_i are drawn with replacement and hence can be repeated. Since repetition is possible, more likely values of L_i (according to $F(L_i)$) will be sampled more times and less likely values of L_i will be sampled fewer times. Hence, the contribution of more likely values of L_i needs to be "drawn" down, and the contribution of less likely values of L_i needs to be "dragged" up. After these adjustments, equation (9) becomes

$$\langle A(L) \rangle = \frac{\sum_{i=1}^{N} e^{-\beta E(L_i)} A(L_i)/F(L_i)}{\sum_{i=1}^{N} e^{-\beta E(L_i)}/F(L_i)} \tag{10}$$

If $F(L_i) = e^{-\beta E(L_i)}$, then the equation (10) becomes

$$\langle A(L) \rangle = \frac{\sum_{i=1}^{N} A(L_i)}{N} = \frac{1}{N} \sum_{i=1}^{N} A(L_i) \tag{11}$$

Hence, if we draw L_i from $e^{-\beta E(L_i)}$, then $\langle A(L) \rangle$ is the just the average of $A(L_i)$ from each draw. The method to draw L_i from $e^{-\beta E(L_i)}$ is described in the next section.
Note that up until this point, we have assumed $A(L_i)$ to be an arbitrary value to be observed. In this project, $A(L_i)$ are $E(L_i)$, $|M(L_i)|$, $E(L_i)^2$ and $M(L_i)^2$ which are then used to calculate the average energy per spin, average absolute magnetization per spin, average heat capacity and average susceptibility.

3 Algorithm Design

From the previous section, it is clear that to calculate $\langle A(L) \rangle$, we need to draw spin configuration samples (L_i) from the probability distribution $e^{-\beta E(L_i)}$ and then perform an average of $A(L_i)$ over all drawn samples. In this project, Monte Carlo Markov Chain and Metropolis-Hastings algorithm is used to draw the spin configuration samples which is an iterative algorithm to draw L_i. Given a spin configuration L_i, we perform random mutations on this spin configuration to get a new configuration L_j. The transition probability from configuration L_i to L_j is defined as $W(L_i \to L_j)$. Similarly, transition probability from L_j to L_i is defined as $W(L_j \to L_i)$. The probability of configuration L_i and L_j is $P(L_i)$ and $P(L_j)$ respectively.

In Monte Carlo Markov Chain processes (like this one), the probability of going out of a configuration L_i should be equal to the probability of going into the configuration L_j. This is called detailed balance and is a necessary condition for the samples to converge to the probability distribution. Mathematically,

$$P(L_i)W(L_i \to L_j) = P(L_j)W(L_j \to L_i) \tag{12}$$

Taking $P(L_i) = e^{-\beta E(L_i)}$ from equation (5),

$$e^{-\beta E(L_i)}W(L_i \to L_j) = e^{-\beta E(L_j)}W(L_j \to L_i) \tag{13}$$

$$\frac{W(L_i \to L_j)}{W(L_j \to L_i)} = e^{\beta(E(L_i)-E(L_j)} \tag{14}$$

Setting $\Delta H = E(L_j) - E(L_i)$, and $W(L_j \to L_i) = 1$ since the choice is arbitrary,

$$W(L_i \to L_j) = e^{-\beta \Delta H} \tag{15}$$

Hence, if $\Delta H \leq 0$, then the transition from L_i to L_j is taken with probability 1. However, if $\Delta H > 0$, then the transition from L_i to L_j is taken with probability $e^{-\beta \Delta H}$. If the transition is taken, then the new configuration becomes L_j, otherwise, the configuration L_i remains the same. Then, the process is repeated by taking the result of the previous transition as the new initial configuration and taking a transition to another configuration L_k. Note that for each configuration, just one random mutation is performed to test the transition to another configuration. Hence, to make sure that each L_i is sufficiently distinct from the previous one and that the samples are uncorrelated, multiple transitions from L_i are "grouped" as just one transition. Algorithm 1 describes the algorithm more clearly.
Regardless of "grouping" or not, we can obtain an arbitrary number of configurations L_i using this method, and from equation (9), the error in the estimation of $\langle A(L) \rangle$ decreases as more configurations are used. Now, we generate N_{samples} samples through this process and the average value of an observable $A(L_i)$ becomes

$$\langle A(L) \rangle = \frac{\sum_{i=1}^{N_{\text{samples}}} A(L_i)}{N_{\text{samples}}} \tag{16}$$

.
Additionally, since Monte Carlo Markov Chain methods take multiple iterations to reach the probability distribution, the configurations L_i obtained in the initial iterations need to be thrown away, and not included in computing $\langle A(L) \rangle$ in equation (16). Let the number of samples thrown away be $N_{\text{throwaway}}$. Then, equation (16) takes the form

$$\langle A(L) \rangle = \frac{\sum_{i=N_{\text{throwaway}}}^{N_{\text{samples}}} A(L_i)}{(N_{\text{samples}} - N_{\text{throwaway}})}$$

The above steps can be summarized in the Algorithm (1) and (2). Before the algorithm is started, a running sum of each observable is maintained (for computing the average). In this project, the observables are energy per spin, energy squared per spin, magnetism per spin, magnetism squared per, and absolute magnetism per spin. Each of these observables can be represented by a corresponding $A(L_i)$:

$$A(L) \text{ for energy} = E(L) \tag{17}$$

$$A(L) \text{ for energy squared} = E(L)^2 \tag{18}$$

$$A(L) \text{ for magnetism} = M(L) \tag{19}$$

$$A(L) \text{ for absolute magnetism} = |M(L)| \tag{20}$$

$$A(L) \text{ for magnetism squared} = M(L)^2 \tag{21}$$

Note that $A(L)$ mentioned above are for the entire lattice and need to be divided by the lattice size at the end to get observable per spin.

The Monte Carlo Markov Chain algorithm is divided into two parts - Metropolis Step and the Markov Step. In the Metropolis Step, spin flip of a random point on the lattice is proposed and performed through the discussion before. In the Markov Step, the Metropolis Step is conducted multiple times, and a running sum of each observable (from multiple Metropolis steps) is maintained.

Algorithm 1 Monte Carlo Markov Chain Ising Model - Metropolis Step

1: Start with a spin configuration L_i. Calculate the energy of this configuration $E(L_i)_i$.
2: Take a random point on the lattice and calculate the final energy $E(L_i)_f$ if a flip at this point is conducted.
3: Calculate $\Delta H = E(L_i)_f - E(L_i)_f$.
4: **if** $\Delta H \leq 0$ **then**
5: The flip is conducted
6: **else**
7: Draw random value u from uniform distribution U(0,1)
8: **if** $u \leq e^{-\beta \Delta H}$ **then**
9: The flip is conducted
10: **end if**
11: **end if**

Algorithm 2 Monte Carlo Markov Chain Ising Model - Markov Step

Require: $n = 1$

Start with an initial state configuration L_i
$E_{\text{sum}} \leftarrow E(L_i)$
$E_{\text{squared, sum}} \leftarrow E(L_i)^2$
$M_{\text{absolute, sum}} \leftarrow |M(L_i)|$
$M_{\text{squared, sum}} \leftarrow M(L_i)^2$
$norm \leftarrow (N_{\text{samples}} - N_{\text{throwaway}}) \times$ Lattice Size
while $n \leq N_{\text{samples}}$ **do**
    $L_{temp} \leftarrow L_i$
    metrop$_{idx} \leftarrow 1$
    while metrop$_{idx} \leq N_{\text{Metropolis Steps}}$ **do**
        $L_{temp} \leftarrow$ Algorithm 1 (Metropolis Step) on L_{temp}
        metrop$_{idx} \leftarrow$ metrop$_{idx} + 1$
    end while
    $L_i \leftarrow L_{temp}$
    if $n \geq N_{\text{throwaway}}$ **then**
        $E_{\text{sum}} \leftarrow E_{\text{sum}} + E(L_i)$
        $E_{\text{squared, sum}} \leftarrow E_{\text{squared, sum}} + E(L_i)^2$
        $M_{\text{absolute, sum}} \leftarrow M_{\text{absolute, sum}} + |M(L_i)|$
        $M_{\text{squared, sum}} \leftarrow M_{\text{squared, sum}} + M(L_i)^2$
    end if
    $n \leftarrow n + 1$
end while
$\langle E \rangle \leftarrow E_{\text{sum}}/norm$
$\langle E^2 \rangle \leftarrow E_{\text{squared, sum}}/norm$
$\langle |M| \rangle \leftarrow M_{\text{absolute, sum}}/norm$
$\langle M^2 \rangle \leftarrow M_{\text{squared, sum}}/norm$

From the algorithm, we get the values of $\langle E \rangle$, $\langle E \rangle$, $\langle |M| \rangle$, and $\langle M^2 \rangle$ for a fixed value of temperature T. The average heat capacity per spin and average susceptibility per spin is calculated at the end as

$$\text{Average Heat Capacity Per Spin: } C = \frac{\partial E}{\partial T} = \frac{(\Delta E)^2}{k_b T} = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_b T^2} \tag{22}$$

$$\text{Average Susceptibility Per Spin: } X = \frac{\partial E}{\partial T} = \frac{(\Delta M)^2}{k_b T} = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_b T^2} \tag{23}$$

Again, let A denote any observable: $\langle E \rangle$, $\langle E \rangle$, $\langle |M| \rangle$, $\langle M^2 \rangle$, C, and X. Now, the procedure is repeated for different values of temperature $T \in \tau = \{T_1, T_2, T_3 \dots T_K\}$ and for each temperature, the average value $\langle A \rangle$ is recorded. Hence, a set $\{\langle A \rangle(T_1), \langle A \rangle(T_2) \dots \langle A \rangle(T_K)\} = \alpha_A(T)$ for each observable is obtained, with entries in this set corresponding to the average value of the observable for a temperature. To check for phase transitions for an observable, sudden change in the entries $\alpha_A(T)$ is investigated. It is expected that the sudden change occurs near the Curie Temperature ($T_c = 2.27$)
Note that for each observable, the set $\alpha_A(T)$ corresponds to the value of that observable obtained across multiple temperatures. Hence, for a set $\alpha_A(T)$ best-fit function can be calculated that best models $\alpha_A(T)$ as a function of temperature. For example, $\alpha_A(T)$ might correspond to numerically calculated average absolute magnetism per spin at different values of temperature, and a best-fit function

is calculated that best models the obtained values of average absolute magnetism per spin as a function of temperature.
Since different observables have different dependencies on temperature, the relationship between the obtained average values of the observable and the temperature is visually studied, and then a parameterized function is chosen which could model this relationship. Next, the best-fit parameters of this parameterized function are calculated which minimizes the mean squared error between the obtained average values and predicted values from the model.

4 Results

In this section, the result of the Ising Model simulation for each observable (as a function of temperature) is presented and a best-fit model to describe the relationship is also provided. Additional qualitative analysis is provided at the phase transition. The lattice size for the model was chosen to be $16 \times 16 = 256$. The temperature was varied from 0.1 to 6 with a step of 0.31, hence, a total of 20 temperature points. The number of samples $N_{\text{samples}} = 20000$, out of which $N_{\text{throwaway}} = 7000$ are thrown away and are not included in computing average observables. Additionally, $N_{\text{Metropolis Steps}} = 16 \times 16/2$

4.1 Average Energy Per Spin

The red line in Figure 1 shows the plot of observed average energy per spin and temperature. It can be seen that near the Curie Temperature, ($T = 2.27$) the value of average energy per spin significantly changes, suggesting a phase shift.

From equations (3) and (2), it can be observed that the least possible energy per spin is -2 and occurs when all the lattice points have the same spin. From the graph, it can be observed that when the temperature is below the Curie Temperature, then the energy per spin is around -2 which suggests that spin configuration is mostly parallel (most points have the same spin) at lower temperatures. As the temperature increases, the energy per spin is also observed to increase which is caused by the spin configuration breaking parallel alignment. This can be explained by the fact that as the temperature increases, the probability of spin flip for $\Delta H > 0$ in equation (15) increases. Hence, the spin flips which cause energy gain become more probable at high temperatures. The graph also supports this argument since at high temperatures, the average energy per spin increases which can be explained by the increased number of "energy-increasing spin flips".

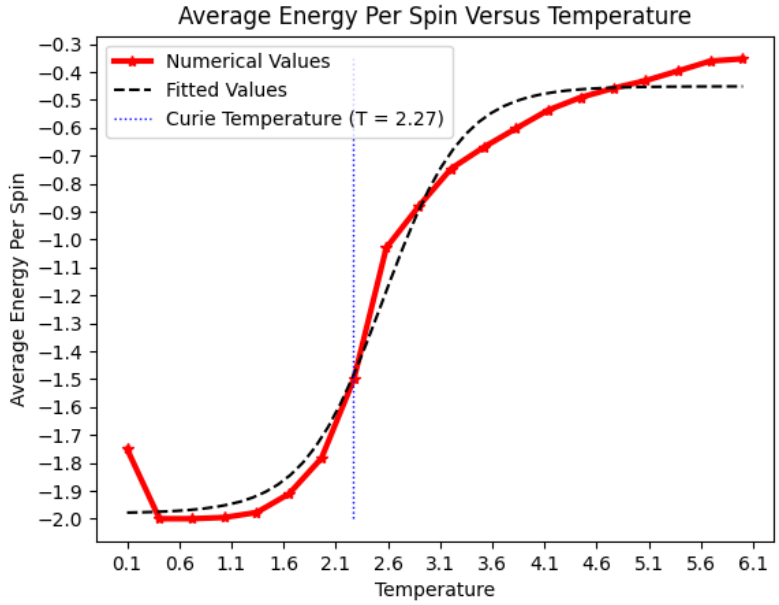

Figure 1: The red plot shows the average energy per spin observed at various temperatures. Each red star marker corresponds to numerically obtained values of average energy per spin at a given temperature which is then interpolated. The blue dotted line corresponds to the Curie Temperature $T = 2.27$, and the black dashed line corresponds to the best-fit model.

The red plot suggests that the relationship between average energy per spin and temperature could be modeled as a sigmoid function. A sigmoid function $\sigma(x)$ is given as

$$\sigma(x) = \frac{1}{1 + e^{-x}} \tag{24}$$

The sigmoid function has been modified to add offset and scaling parameters in the x and y directions. After adding these parameters, $\sigma(x)$ becomes

$$\sigma(x) = y_{\text{offset}} + \frac{y_{\text{scale}}}{1 + e^{-(x - x_{\text{offset}})/x_{\text{scale}}}} \tag{25}$$

The relationship between energy per spin and temperature is modeled as

$$E(T) = E_{\text{offset}} + \frac{E_{\text{scale}}}{1 + e^{-(T - T_{\text{offset}})/T_{\text{scale}}}} \tag{26}$$

Using the notation from the previous section, let the observed values of average energy per spin be represented by the set $\alpha_E(T)$ where $T \in \tau$. The mean squared error between these numerical values and predicted values (from the parameterized function) of average energy per spin becomes

$$g(E_{\text{offset}}, E_{\text{scale}}, T_{\text{offset}}, T_{\text{scale}}) = \sum_{T \in \tau} (E(T) - \alpha_E(T))^2 \tag{27}$$

The values of $E_{\text{offset}}, E_{\text{scale}}, T_{\text{offset}}, T_{\text{scale}}$ which minimize $g(E_{\text{offset}}, E_{\text{scale}}, T_{\text{offset}}, T_{\text{scale}})$ are found. The black dashed line in Figure 1 shows the best-fit model of the modified sigmoid function that minimizes the mean-squared error in equation (27). It can be noticed that the modified sigmoid function models

the "middle" temperature ranges $1.10 < T \leq 3.10$ well but fails to model the energy near the edges. This can be explained by the existence of a statistic anomaly at $T = 0.1$ which causes the tail of the distribution to be modeled incorrectly. Additionally, the numerically obtained values of average energy per spin do not reach a constant upper bound for the used temperature range as they still seem to increase even at $T = 5.6$ and $T = 6.1$, and thus it fails to model the numerically obtained values of average energy per spin.

4.2 Average Absolute Magnetism Per Spin

The red line in Figure 2 shows the plot of average absolute magnetism per spin and temperature. It can be seen that at lower temperatures ($0.1 \leq T \leq 2.27$), the material is ferromagnetic. This can be explained from the previous discussion in "Average Energy Per Spin (4.2)": since the spin configuration favors parallel spin alignment at lower temperatures, the spins add up and an absolute magnetism is observed. However, as the temperature increases, the anti-parallel spin configurations become more probable which decreases the absolute magnetism. Thus, the absolute magnetism approaches zero as temperature increases.

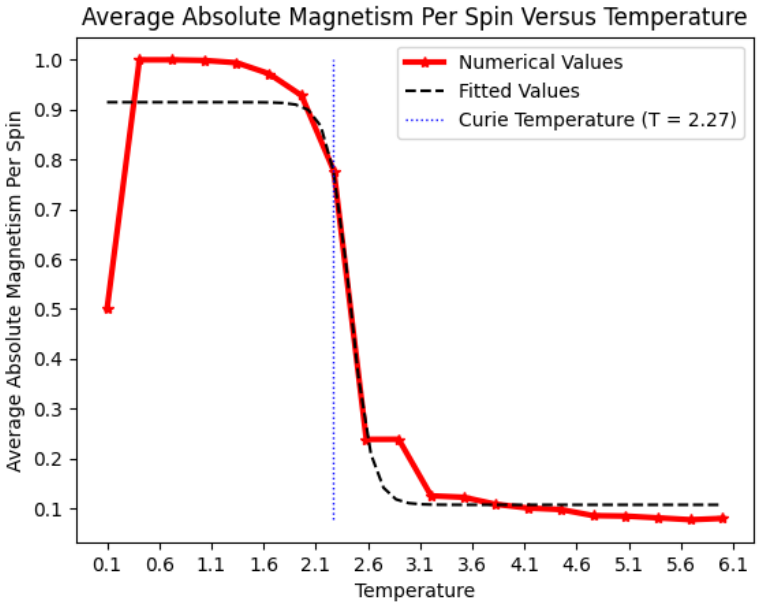

Figure 2: The red plot shows the numerically obtained values of absolute magnetism per spin observed at various temperatures. Each red star marker corresponds to an observed value of average absolute magnetism per spin at a given temperature which is then interpolated. The blue dotted line corresponds to the Curie Temperature $T = 2.27$, and the black dashed line corresponds to the best-fit model.

Similar to the relationship between average energy per spin and temperature, the plot suggests that the relationship between average absolute magnetism per spin and temperature is also sigmoid. The black dashed line in Figure 2 shows the best-fit model of the modified sigmoid function that minimizes the mean-squared error between the observed values and predicted values of average absolute values per spin.

For absolute magnetism, the sigmoid model fails to model absolute magnetism at temperature $T < T_c$ as absolute magnetism should be predicted as 1 (based on observed values and physical restrictions),

but the sigmoid predicts it as less than 1. This could be explained by the fact that there is an outlier at $T = 0.10$ which is a statistical anomaly (as the average absolute magnetism per spin is 0.5). However, since the mean-squared error approach gives equal weight to each data point, the sigmoid function "tries" to capture the first data point and causes the predictions at $T < T_c$ to be less than 1.

4.3 Average Heat Capacity Per Spin

The red line in Figure 3 shows the plot of average heat capacity per spin and temperature. It can be seen that the average heat capacity per spin is zero at lower temperatures, but increases rapidly as the temperature approaches Curie Temperature ($T = 2.27$) and then drops as the temperature is further increased.

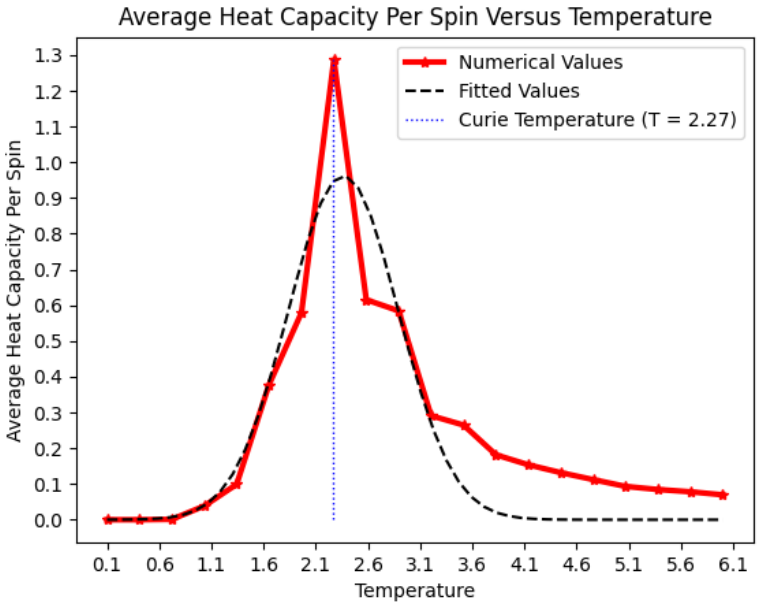

Figure 3: The red plot shows the average heat capacity per spin observed at various temperatures. Each red star marker corresponds to the observed value of heat capacity per spin at a given temperature which is then interpolated. The blue dotted line corresponds to the Curie Temperature $T = 2.27$, and the black dashed line corresponds to the best-fit model.

The plot suggests that the relationship between average heat capacity per spin and temperature can be modeled as a Gaussian function. The modified Gaussian function (with scaling and shifting parameters) used as a model is given as:

$$C(T) = \frac{C_{\text{scale}}}{T_{\text{scale}}} exp\left(-\frac{1}{2}\left(\frac{T - T_{\text{offset}}}{T_{\text{scale}}}\right)^2\right) \tag{28}$$

If the measured values of heat capacity per spin are represented by the set $\alpha_C(T)$ where $T \in \tau$, then the mean squared error as a function of $C_{\text{scale}}, T_{\text{offset}}, T_{\text{scale}}$ is given as

$$g(C_{\text{scale}}, T_{\text{offset}}, T_{\text{scale}}) = \sum_{T \in \tau} (C(T) - \alpha_C(T))^2 \tag{29}$$

The values of $C_{\text{scale}}, T_{\text{offset}}, T_{\text{scale}}$ which minimize $g(C_{\text{scale}}, T_{\text{offset}}, T_{\text{scale}})$ are found. The black dashed line in Figure 3 shows the best-fit model of the modified Gaussian function that minimizes the mean-squared error between observed and predicted values of average heat capacity per spin.
It can be observed that while this modified Gaussian function gets the general trend of the relationship correct, it does not capture important specific features. For example, heat capacity increases to 1.3 at the Curie Temperature but since the mean-squared error is used (which assigns equal weight to each data point), it does not capture the peak and predicts the heat capacity to be less than 1.3.
Additionally, the asymmetric nature is not modeled. For example, from temperature 0.1 to T_c, heat capacity increases rapidly but declines slowly with a further increase in temperature from T_c to 6.0. Since Gaussian is symmetric, it does not capture the asymmetric rise and fall correctly.

4.4 Average Susceptibility Per Spin

The red line in Figure 4 shows the plots of average susceptibility per spin and temperature. At lower temperatures, the susceptibility is near zero, however, as the temperature approaches Curie Temperature ($T = 2.27$), the susceptibility increases rapidly to near 6.5 and then decreases as the temperature increases further.

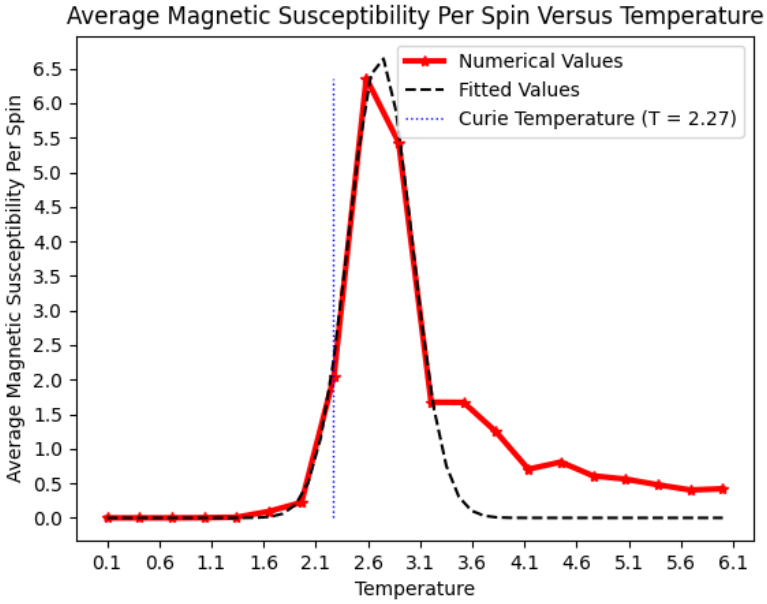

Figure 4: The red plot shows the average magnetic susceptibility per spin observed at various temperatures. Each red star marker corresponds to the observed value of average magnetic susceptibility per spin at a given temperature which is then interpolated. The blue dotted line corresponds to the Curie Temperature $T = 2.27$, and the black dashed line corresponds to the best-fit model.

Similar to the relationship between average heat capacity per spin and temperature, the plot suggests that the relationship between average susceptibility per spin and temperature can also be modeled with a parameterized Gaussian function. The black dashed line in Figure 4 shows the best-fit model of the modified Gaussian function that minimizes the mean squared error between observed and predicted values of average susceptibility per spin

Contrary to the problem with the Gaussian model with heat capacity, the Gaussian model captures

the peak of magnetic susceptibility effectively. However, similar to average heat capacity per spin, there exists an asymmetric nature of the relationship of susceptibility with temperature which cannot be captured by the current modified Gaussian model since it can only model symmetric relationships.

5 Conclusion

In this project, Ising Model was simulated and the average energy per spin, absolute magnetism per spin, heat capacity per spin, and susceptibility per spin were calculated for varying temperature ranges. Additionally, these properties were analyzed for phase transition near the Curie temperature, and best-fit functions were calculated to model these physical functional properties as a function of temperature, and additional analysis was provided on what parts of the observed data set these best-fit models fail to model correctly.

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