Physics 905: 2D Ising Model

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Abstract

The complete 2D Ising Model is computationally expensive to solve because it requires calculating many states. This calculation is simplified in this study by using the Metropolis Algorithm, which is a Monte Carlo Method. The calculated Curie Temperature is around 2.5 $\frac{J}{k_B}$ which is close to the exact solution of about 2.3 $\frac{J}{k_B}$.

1 Introduction

The 2D Ising model is a mathematical model of the magnetization of a 2D lattice with periodic boundary conditions where the spin at each point, atom, in the lattice is either up (+1) or down (-1). The magnetization is calculated using Equation 1, where N is the number of atoms and s_i^{state} is the spin at a particular point (i) and in a particular state. The partition function (Z) and β are defined by Equations 2 and 3, respectively.

$$m = \frac{1}{N}\sum_{i=1}^{N}\sum_{states}\frac{s_i^{state}e^{-\beta\epsilon_{state}}}{Z} \tag{1}$$

$$Z = \sum_{states} e^{-\beta\epsilon_{state}} \tag{2}$$

$$\beta = \frac{1}{k_B T} \tag{3}$$

The Curie Temperature (T_C) is the temperature where the magnetization drops to zero. The exact solution to the 2D Ising Model has been solved by Lars Onsager[1] and used to calculate the Curie Temperature to be about 2.269 $\frac{J}{k_B}$. However, this is a computationally difficult problem to solve because the number of possible states is 2^N and using 2^N states would take a long time to complete the calculation. Therefore, the following study uses a Monte Carlo method called the Metropolis Algorithm to strategically randomly sample states and thus simplify the calculation to find the Curie Temperature.

2 Computational Details

This project was done using the Monte Carlo method known as the Metropolis Algorithm. The starting system was a square system with 100x100 points. Each point was initialized to be spin up (+1). A point was then chosen at random and the spin (s_i) was flipped by multiplying the value by negative one. Whether the randomly chosen spin should stay flipped or be flipped back was decided by the Metropolis test. If the change in energy, $\delta\epsilon$ in Equation 4, of the system was negative the than the new state is kept. If the change in energy of the system is positive, then a fraction, R, is randomly chosen. If the condition in Equation 5 is true the new state is not kept and the system is changed back to the old state. However, if the change in the energy of the system is positive and the condition in Equation 5 is not met the new state is kept.

$$\delta\epsilon = \epsilon_{new} - \epsilon_{old} \tag{4}$$

$$e^{\frac{-(\epsilon_{new}-\epsilon_{old})}{k_B T}} \lesssim R \tag{5}$$

The energy difference, $\delta\epsilon$, between the energy of the state after the random spin was flipped, ϵ_{new}, and the energy of the state before the random spin was flipped, ϵ_{old}, was calculated using Equation 4 and assuming J=1. The energies of the states were calculated, as shown in Equation 6, using only the $\langle i, j\rangle$ bonds which changed when the randomly chosen spin was flipped. Thus when the energy values were calculated only the bonds between the spin which was changed and the four neighboring spins were considered.

$$\epsilon = H = -J \sum_{\langle i,j \rangle} s_i s_j \tag{6}$$

The process of flipping the spin and applying the Metropolis Test was iterated for 5x10^6 spins, a sufficient number for convergence as determined and described in the following section, using the microcanonical ensemble at each dimensionless temperature ($k_B T/J$) between 1.0 and 4.0. Every integer value of dimensionless temperature between 1.0 and 4.0 was analyzed as well as temperatures with an increment of 0.1 between 2.0 and 3.0. The dimensionless values between 2.0 and 3.0 were analyzed at a smaller increment because the exact solution to the Ising Model is about 2.3 J/k_B and therefore it was assumed that the Curie Temperature calculated by the algorithm developed here would be in the range of 2 to 3 J/k_B. After every one hundred iterations the magnetization, m, was calculated using Equation 7, where N is the number of spins in the system, 10000 in this work.

$$m = \left| \frac{1}{N} \sum_{i=1}^{N} \langle s_i \rangle \right| \tag{7}$$

The iterations between 3x10^6 and 5x10^6, a range where convergence was seen for all dimensionless temperature values, was split into 20 sections of 100000 consecutive spin flips and an average m value for each of these 20 sections was then calculated. The 20 averaged m values for each dimensionless temperature were then averaged and the averages/standard deviations were plotted to determine the Curie temperature, T_C.

3 Results and Discussion

The developed algorithm was run for 7x10^6 iterations at each dimensionless temperature (k_BT/J) to determine how many iterations were necessary for the magnetization, m, to converge at every dimensionless temperature value, Figure 1.

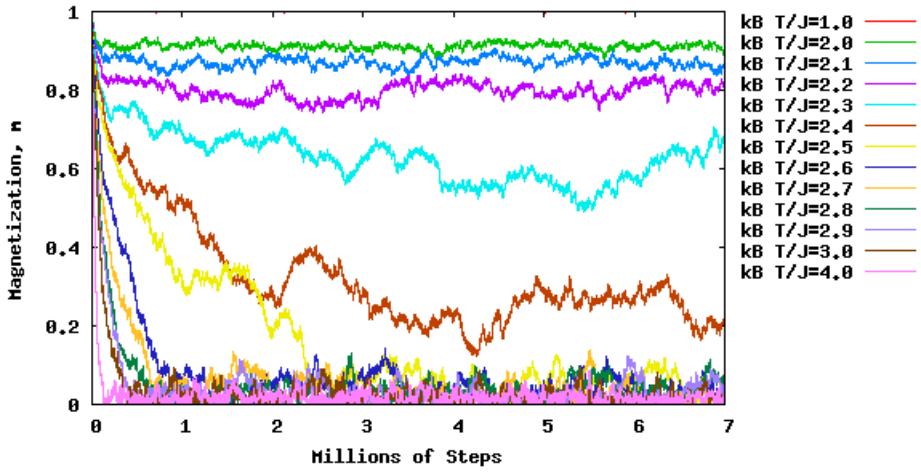

Figure 1: The calculated magnetization, m, over a total of seven million steps for each of the dimensionless temperatures analyzed.

Figure 1 shows that when the temperature value is significantly larger or smaller than T_C the m value converges quickly. However, when the temperature value is close to T_C the m value takes significantly more iterations to converge. The dimensionless temperature which took the most iterations to converge was 2.5, Figure 2.

From Figure 2 it was determined that around 2.5 million steps are required for the m value of the dimensionless temperature value of 2.5, and thus every dimensionless temperature, to converge. Therefore, when computing the average m values to determine the Curie Temperature the m values of the iterations between 3x10^6 and 5x10^6 were used to ensure the range was high enough that the m values used were converged.

The developed algorithm was then run for 5x10^6 iterations, Figure 3, and

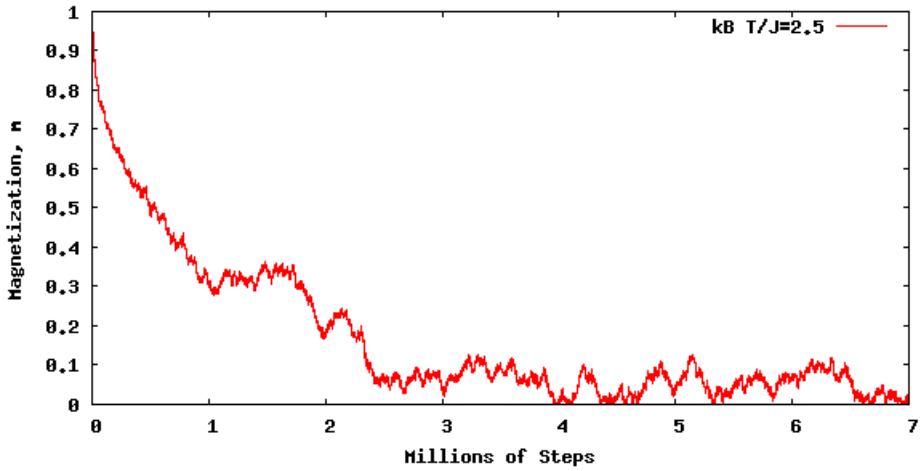

Figure 2: The magnetization, m, for only the dimensionless temperature 2.5 over 7 million steps. This was the dimensionless temperature which took the most steps to converge.

the average m values were plotted with their corresponding standard deviations, Figure 4.

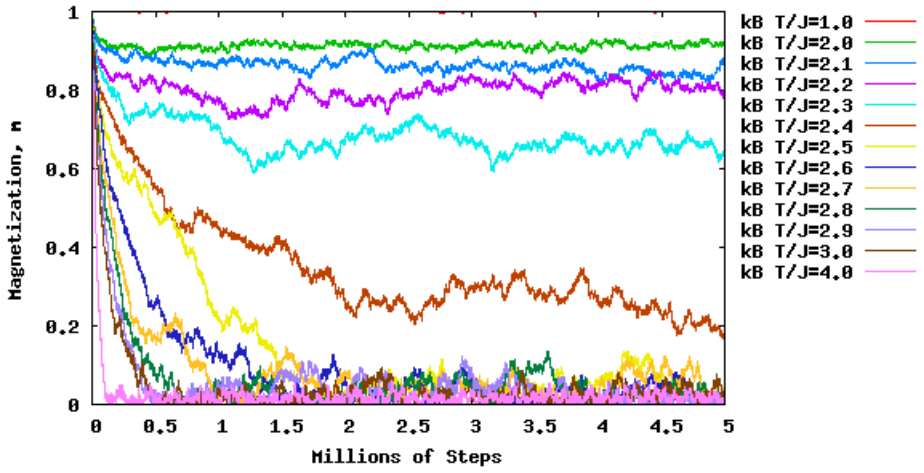

Figure 3: The magnetization calculated for various dimensionless temperatures, k_BT/J, for five million time steps.

From Figure 4 it is apparent that the calculated T_C value is about 2.5 J/k_B. This value is close to the T_C of 2.269 J/k_B obtained from the exact solution solved by Onsager[1].

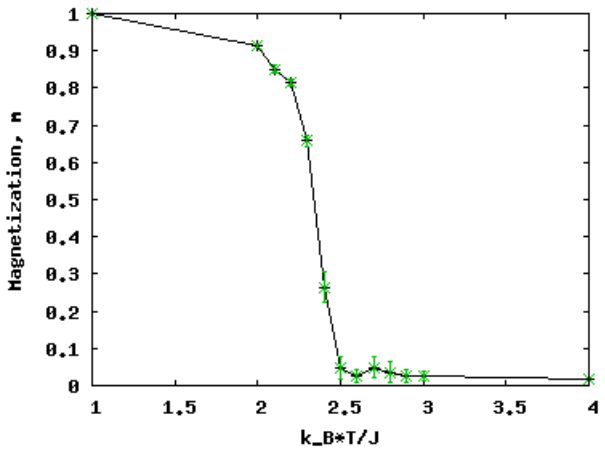

Figure 4: The average magnetization at various dimensionless temperatures, k_BT/J.

4 Conclusion

Through using the Metropolis Algorithm the T_C was calculated to be about 2.5 J/k_B. This appears to be a good approximation since the exact solution solved by Onsager[1] is 2.269 J/k_B. However, it is a simplified model and therefore is not as accurate as the exact solution.

5 References

(1) Onsager, L., *Physical Review 65* (3/4), 117-149, **1944**.