PHSX815_Project4:
Estimation of Critical Temperature for Magnetic Phase Transition using 2D Ising model simulated by Monte Carlo Metropolis Algorithm

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1 Introduction

Ferromagnets belong to the class of materials that can retain magnetization even in the absence of external magnetic field. This kind of materials demonstrate long-range ordering of atoms and form domains where unpaired electrons have identical spins. In non-magnetic substances, the domains with opposite alignment cancel out each others field which results in net zero magnetization. When magnetic materials are heated to higher temperatures, the thermal motion competes with the tendency of dipoles to align and if the temperature is increased to a value called Critical Temperature (T_c), second-order phase transition occurs where the system becomes unable to sustain the spontaneous magnetization.

In order to study this phase transition and estimate the critical temperature, we will use the 2D Ising model for a square lattice of size $L \times L$. The 1D Ising model was solved by Ising in the year 1924 [1] which did not demonstrate any phase transition. But, 2D square-lattice Ising model was solved analytically much later in 1944 by Lars Onsager [2]. According to this model, the expression for the Energy of the system is,

$$H = J \sum_{i=0}^{L-1} \sum_{j=0}^{L-1} (s_{i,j} s_{i,j+1} + s_{i,j} s_{i+1,j}) \tag{1}$$

where J is the strength of interaction between the 2 spins, and $s_i = 1, -1$. The sum $< i, j >$ runs over the nearest neighbours of i.

Similarly, the Magnetization and Specific Heat are given by the expressions below.

$$< M >=< \sum_{i}^{L} s_i > \tag{2}$$

$$C_v = \frac{< E^2 > - < E >^2}{T^2} \tag{3}$$

The second order phase transition occurs at a particular temperature where there is a discontinuity in the plots of M vs T and C_v vs T. Onsager's solution predicts that the T_c value is 2.268 K for a 2D lattice [2]. A typical plot [3] of C_v vs T indicating the T_c is shown below.

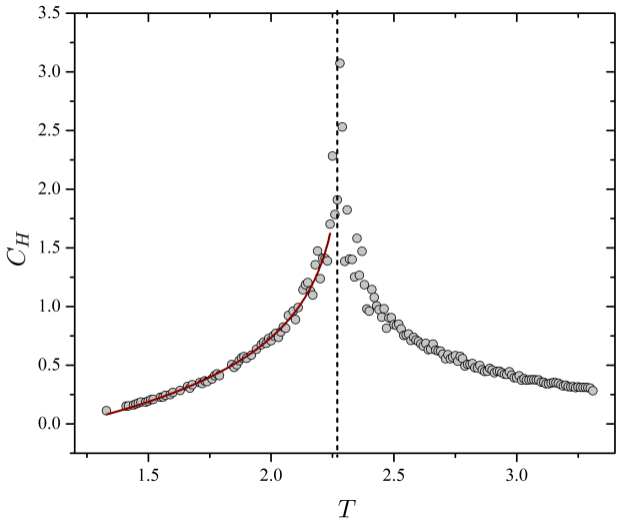


Figure 1: Typical C_v vs T plot for 2D lattice

2 Code and Experimental Simulation

Numerical computations that utilise random numbers are called Monte Carlo methods. In order to generate random numbers we use the standard 'random' library in Python. In order to minimize the free energy of the system we use the Metropolis algorithm. The local energy minima are due to stable orientations of the magnetic domains and some thermal fluctuations are necessary to break them apart and reorder the system to a lower energy state. When the system reaches the global minima, the probability of escaping the configuration is significantly small. The probability of the states are determined by Boltzmann distribution, $P = \exp(-dE/T)$, where, dE is interaction energy between spins assuming periodic boundaries and is simply the difference in energy due to flipping spin i, j. The steps in our algorithm are:

1. Prepare some configurations of N spins.
2. Flip the spin of a randomly chosen lattice site
3. Calculate the change in energy, dE due to spin flipping
4. If the energy change is negative, it is favorable and hence accepted. If the energy change is greater than zero, accept it and assign probability $P = \exp(-dE/T)$.
5. Repeat steps from 2 to 4
6. Calculate physical quantities and generate plots.

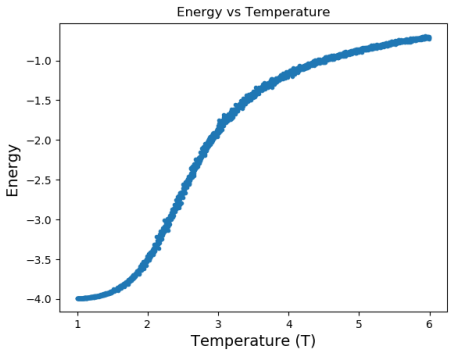
3 Analysis

The question we are trying to answer in this project is, how does the size of lattice and number of MC sweeps affect the calculation of the Magnetisation, Energy and Specific heat of a 2D lattice system and with what accuracy can we estimate T_c by simulating a finite 2D lattice ?

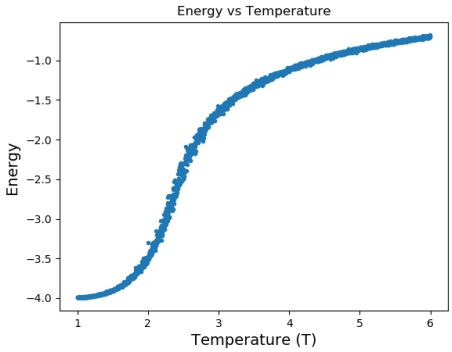
Since, we expect a discontinuity in the plot of specific heat vs temperature at T_c, we will use the temperature corresponding to the maximum value of the C_v as our T_c. Then we will calculate the T_cs for different number of times and fit it to the Gaussian distribution and find expected mean and standard deviation. The fitted mean can be interpreted as the expected value of T_c by our simulation.

3.1 Energy for different lattice parameters and MC sweeps

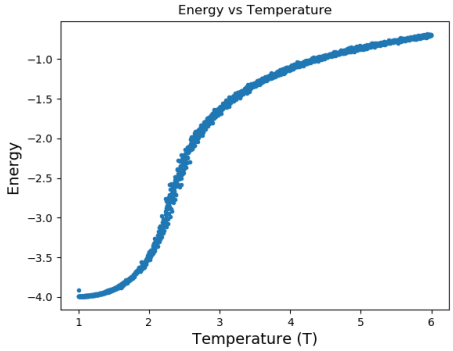
The plots for Energy vs Temperature shows that the calculations for energies at different temperatures are fairly consistent for lattice sizes of 5, 10 and 15 at 100000 MC sweeps. However, the number of MC steps have a significant impact on the fluctuations. The data is more scattered if we reduce the number of MC sweeps to 100 and 1000, even for lattice size of 15×15.



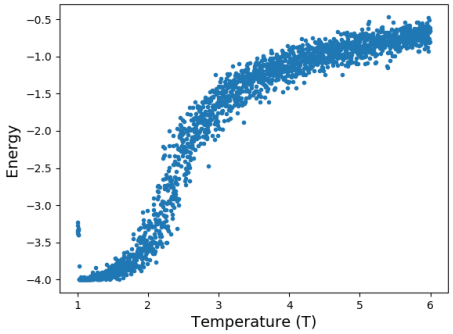
(a) 5×5 lattice and 100000 sweeps



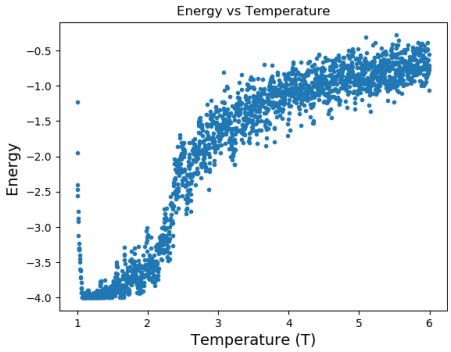
(b) 10×10 lattice and 100000 sweeps



(c) 15×15 lattice and 100000 sweeps



(d) 15×15 lattice and 1000 sweeps

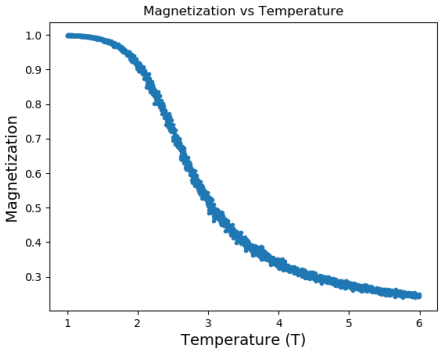


(e) 15×15 lattice and 100 sweeps

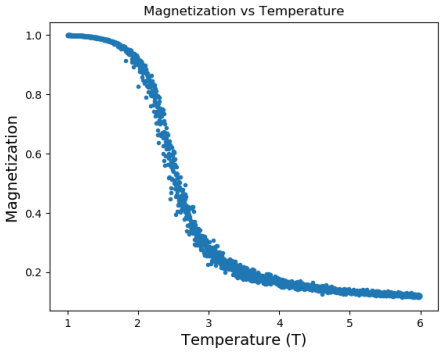
Figure 2: Plots of Energy vs Temperature for different lattice sizes and MC sweeps

3.2 Magnetisation for different lattice sizes and MC sweeps

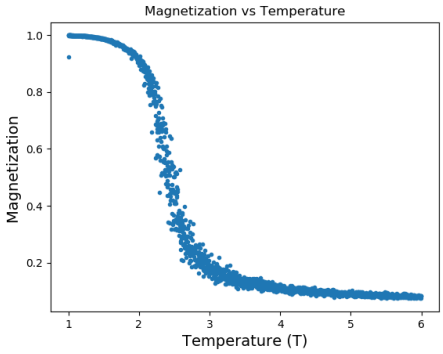
We can visualize the transition occuring at T_c through the plot of Magnetisation vs temperature. At $T-c$, the magnetisation is supposed to rapidly fall from 1 to 0. This is the phase transition from ferromagnetic to paramagnetic system. Unlike in the case of energy plots where the number of lattice did not play significant role, here we can see that as we increase the dimension of our lattice, the transition is more pronounced and occurs within a very narrow range. In reality, there are millions of atoms in the crystals and we do expect that this transition will also be abrupt if we consider higher lattice sizes but it has computational costs associated with it.



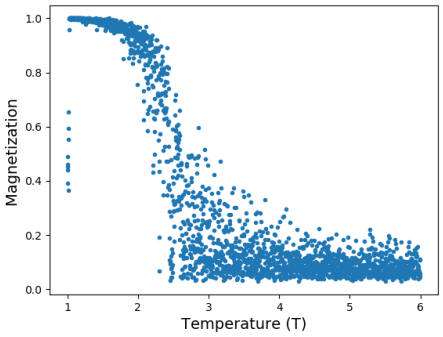
(a) 5×5 lattice and 100000 sweeps



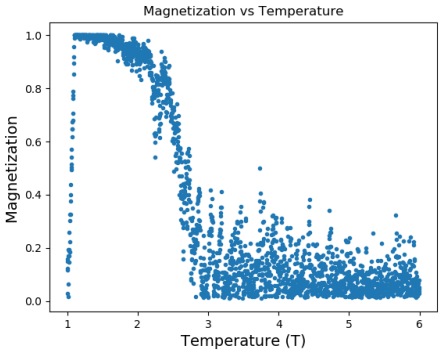
(b) 10×10 lattice and 100000 sweeps



(c) 15×15 lattice and 100000 sweeps



(d) 15×15 lattice and 1000 sweeps

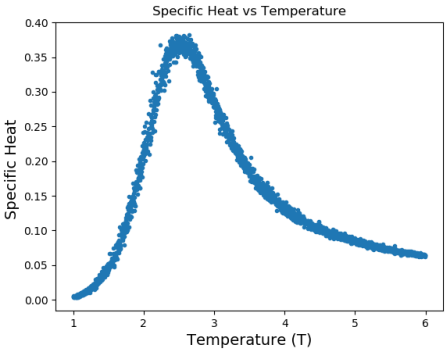


(e) 15×15 lattice and 100 sweeps

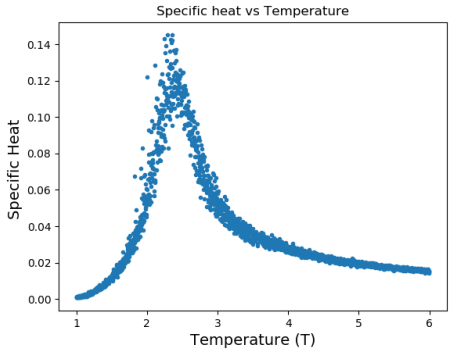
Figure 3: Magnetisation vs Temperature plots for different lattice sizes and MC sweeps

3.3 Specific heat for different lattice parameters and MC sweeps

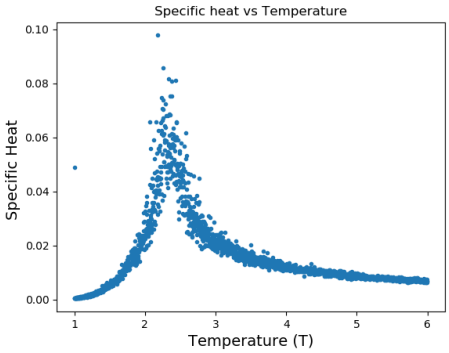
For the purpose of estimating the T_c, we are using the data from the plot of specific heat (C_v vs T. We can notice that there is a discontinuity in the plots at a particular temperature which corresponds to the T_c. In fact, we can clearly see that as we increase the size of lattice, the discontinuity becomes more and more clear. And also, the number of MC sweeps needs to be optimum as well for the discontinuity to be visible.



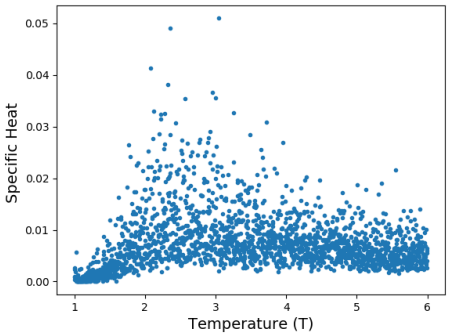
(a) 5×5 lattice and 100000 sweeps



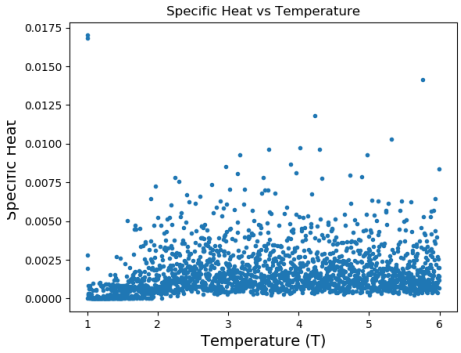
(b) 10×10 lattice and 100000 sweeps



(c) 15×15 lattice and 100000 sweeps



(d) 15×15 lattice and 1000 sweeps



(e) 15×15 lattice and 100 sweeps

Figure 4: Specific Heat vs Temperature for different lattice sizes and MC sweeps

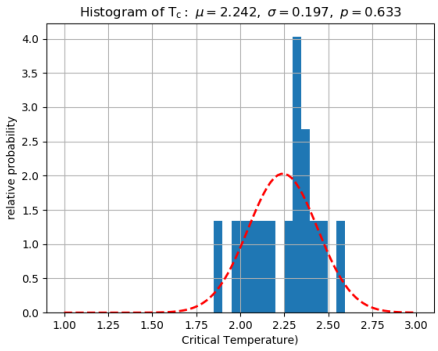
3.4 Error Analysis

Along with the size of the lattice (systematic error), there are many other sources of variation that we have not considered in this experiment. For example, defects (Frenkel defects, Schotky defect, etc.) in the crystals are pretty common and do occur naturally. Likewise, there are also random errors in our experiment due to random disturbances and it does not have a preferred direction. For this project, we are analysing the error due to randomness only.

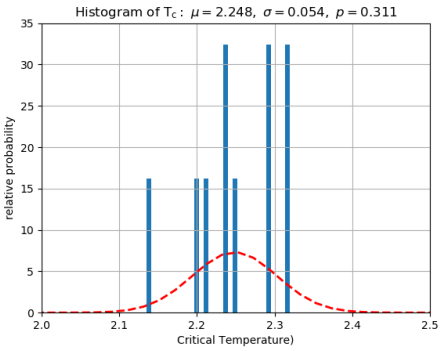
Here we are referring the temperature corresponding to the maxima of C_v s T_c. We are using MC simulation to do our calculations. So, a natural way of determining the error of our estimation would be to run multiple iteration of the same experiment and interpret the average as the estimated parameter

and standard deviation as uncertainty. Also, we expect the distribution of the approximations of the T_c to be gaussian. For this reason, we have fitted the distribution using scipy library. The fit then would give us the expected value of T_c which is also the value that maximizes the likelihood. Finally, we perform two tailed t-test and calculate the p-value for the hypothesis,

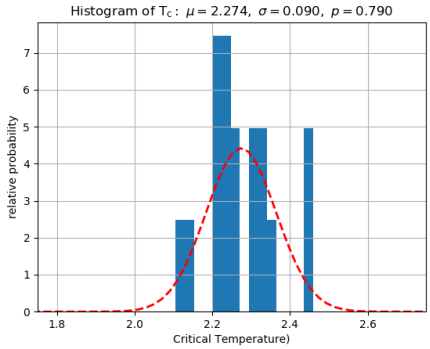
1. $T_c = 2.268K$ i.e H_0
2. $T_c \neq 2.268K$ i.e H_1



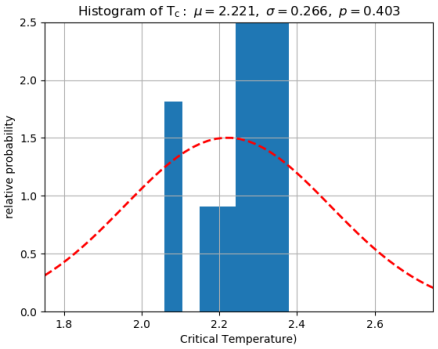
(a) fit using 4 iterations



(b) fit using 10 iterations



(c) fit using 15 iterations



(d) fit using 20 iterations

Figure 5: Gaussian fit of the distribution of T_c for different number of iterations. For those data points that are close by 0.001, we have taken them into the distribution as well. Hence there are more values of T_c than the iteration itself.

From the Figure 4, we can see that our standard deviation is not bad considering we are using small number of iterations only, due to computational limitations. Also, the fit shows that our expected $T - C$ is very close to the theoretical value of 2.268 K. Similary, the p-values are also quite high and we can comfortably reject the alternative hypothesis at 95 percent confidence level. Of course, this does not let us accept the null hypothesis but it does gives us some confidence in our simulation.

We did not calculate the error of each values of the calculated physical quantities due to time limitation. But we could have used the bootstrap method to calculate them. The method is fairly simple which consist of taking N independent measurement of the same quantity several times and then computing quantity as $q = Q/N$ with uncertainty as its standard deviation σ [4].

4 Conclusion

Our Simulations and Analysis reveals that 2D Ising model could explain the magnetic phase transition ocurring in materials. We used different lattice sizes, different numbers of MC sweeps and different number of iterations of the MC simulation to demonsatrate the Phase transition. We saw that in general Lattice size does have a significant role in the determination of the T_c and so does the number of MC sweeps. Along with that, even with the system as small as 20×20 and MC sweeps of 10000, we were able to get fairly close to the predicted T_c value.

References

[1] Ernst Ising. *Beitrag zur Theorie des Ferro-und Paramagnestismus*. PhD thesis, Hamburg, 1924.

[2] Lars Onsager. Crystal statistics. i. a two-dimensional model with an order-disorder transition. *Physical Review*, 65(3-4):117, 1944.

[3] Eduardo Ibarra-García-Padilla, Carlos Gerardo Malanche-Flores, and Freddy Jackson Poveda-Cuevas. The hobbyhorse of magnetic systems: the ising model. *European Journal of Physics*, 37(6):065103, 2016.

[4] Catarina Martins Cosme. Monte carlo methods in critical systems. 2014.