

# Numerical Analysis of 2-D Ising Model

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## **Abstract**

This report is a study of selected properties of ferromagnetic material represented by a two dimensional Ising model using Monte Carlo simulation.

It begins with an introduction of ferromagnetism and the Ising model followed by short notes on the computational techniques implemented. The experimental tasks with results and their analysis are then discussed.

Experimental and analytic solutions for temperature dependence of average magnetization are compared. Critical exponents and critical temperature are found by finite size scaling.

In the end, autocorrelation function of Metropolis algorithm is studied.

## **Acknowledgment**

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## Introduction

Ferromagnetic materials are a class of magnetic materials that form permanent magnets and have many practical applications like electromagnets. The ferromagnetic materials exhibit long range ordering phenomenon at the atomic level which cause the unpaired electron spins to line up parallel with each other in a region called a domain. The domains are randomly oriented with respect to one another in the absence of external field. So although each domain has some net magnetization, there is no total magnetic field observed in the bulk of the sample. When an external magnetic field is applied, the domains already in the direction of the applied field grow at the expense of their neighbors. The spins are all in one direction and a net macroscopic magnetization is observed. The most important property of ferromagnetism is that it retains the magnetism even after the external field has been removed. At temperatures higher than the so called Critical temperature or Curies temperature, a ferromagnetic material undergo second order phase transition into paramagnetic material. The domains now have enough thermal energy to be randomly oriented again. The simplest model that describes ferromagnetic material in two dimensions is the Ising model [1].

The Ising model was invented by the physicist Wilhelm Lenz (1920) and was solved by his student Ernst Ising (1-D Ising model). The 2-D Model (with no applied magnetic field) was solved by L. Onsager (1944). Thermodynamic properties of Ising models in more than three dimensions cannot be solved numerically or analytically.

The Ising model mathematically models a ferromagnetic lattice in statistical mechanics. It consists of discrete variables called the spin. They are arranged in a lattice and each lattice site has only one spin with either +1 (spin up) or -1 (spin down) value. The spins interact only with their nearest neighbors. The Ising model is used to study the phase transitions and cooperative phenomenon [2].

Here we study the 2-D Ising model solved by Onsager. The Hamiltonian,  $H$  of the Ising model is give by:

$$H = -J \sum_{i,j} s_i s_j$$

$J_{ij}$  is the interaction energy between spins at lattice point  $i$  and  $j$ . In case of ferromagnetism, the system will have minimum energy when the spins are all aligned and  $J > 0$ .  $J$  is positive for ferromagnetic material and negative for antiferromagnetic. Here  $i$  and  $j$  run over all lattice sites and are next neighbor pairs.  $s_i$  and  $s_j$  are the spin states at lattice site  $i$  and  $j$  respectively. The parameter  $1/2$  is to avoid double counting. We study the ferromagnetic model in the absence of external magnetic field.

The partition function,  $Z$  of the Ising model is given by:

$$Z = \sum_y e^{-\beta E_y}$$

where  $\beta$  is  $1/(k_B T)$ ,  $T$  is the temperature and  $E_y$  is the energy of the state  $y$ .

## Computational Techniques

- Monte Carlo

Monte Carlo methods are those which solve a problem by generating suitable random numbers and observing that fraction of the numbers obeying some property or properties. The method is useful for obtaining numerical solutions to problems which are too complicated to solve analytically. It was named “the Monte Carlo method” by S. Ulam after the Monte Carlo Casino based on random number generation [3].

There is no single Monte Carlo method but a large class of approaches following a particular pattern [4]:

1. Defining phase space - a domain of possible inputs.
2. Sampling- generating inputs randomly from the phase space using a certain specified probability distribution.
3. Deterministic computation- computing the problem using the generated inputs (random numbers).
4. Final result- aggregation of the individual computation results.

We study the system in thermal equilibrium so that its bulk properties (intensive and extensive) remain unchanged. The probability  $P(x)$  of the system in state  $x$  is then given by normalized Boltzmann factor as [4]:

$$P(x) = \frac{1}{Z} e^{-\beta E_x}$$

where  $\beta = 1/(k_B T)$ ,  $T$  = temperature,  $k_B$  = Boltzmann constant =  $1.380658 \times 10^{-23}$  J/K [##] and  $E_x$  = energy of state  $x$ .

$Z = \sum_Y e^{(-\beta E_Y)}$  = partition function, where  $Y$  represents all possible states of the system with  $E_Y$  corresponding to the energy of the  $Y$ th state.

- Metropolis Algorithm

The Metropolis algorithm is one of the procedures that realize Importance sampling. It involves the construction of a state  $x_{l+1}$  from the previous state  $x_l$  with a transition probability  $W(x_l \rightarrow x_{l+1})$ . Here many Markov chains are constructed from one Markov chain. We choose  $W$  in such a way that the probability distribution of the states tends towards the equilibrium probability for infinite number of states [4].

In our project we choose the transition probability from state  $x_l$  to  $x_{l'}$  as:

$$W(x_l \rightarrow x_{l'}) = \begin{cases} \frac{1}{\tau_s e^{-\frac{\partial H}{k_B T}}} \\ \frac{1}{\tau_s} \end{cases}$$

where  $\tau_s$  is an arbitrary factor and we choose it to be unity.

The algorithm for spin flip is given as the following:

1. Set all the macroscopic variables like the lattice length  $L$ .
2. Select the lattice site  $i$  where the spin  $S_i$  is to be flipped.
3. Calculate the energy difference ( $\partial H$ ) associated with this spin flip.
4. Choose a random number  $Z$  between zero and unity.
5. Only if  $Z < \tau_s W$ , the spin is flipped. The end of this step gives a new configuration which may or may not have the spin flipped.
6. The above steps are repeated a number of times

- **Finite Size Scaling**

We are studying a statistical system which is defined at thermodynamic limit i.e.  $L \rightarrow \infty$ , but due to computational limitations the system has finite lattice size  $L \times L$ . The correlation length  $\xi(t)$  at  $T \gg T_c$  and at  $T \ll T_c$  is small and the system is comparable to an infinite system. But at  $T \approx T_c$ , the correlation length becomes equivalent to the length  $L$  of the system. As a result the critical exponents at  $T_c$  get rounded and shifted. Thus we need to do finite size scaling which determines the “real” critical singularities by observing the measured quantities for different lengths (sizes) of the system [4].

The following relations define the critical exponents-  $\beta, \gamma, \alpha$  and  $\nu$  and are valid only close to the critical temperature:

$$\begin{aligned} m_L(t) &= L^{-\beta/\nu} \cdot \tilde{m}(L^{1/\nu} \cdot t) \\ \chi_L(t) &= L^{\gamma/\nu} \cdot \tilde{\chi}(L^{1/\nu} \cdot t) \\ c_L(t) &= L^{\alpha/\nu} \cdot \tilde{c}(L^{1/\nu} \cdot t) \end{aligned} \quad \text{-equation} \quad (1)$$

$$t = \frac{T - T_c}{T_c}$$

where  $m_l$ ,  $\chi_l$  and  $c_l$  are spontaneous magnetization, susceptibility and specific heat respectively,  $L$  is the lattice length and  $(\tilde{\chi}, \tilde{c}, \tilde{m})$  are called the scaling functions. The scaling functions are independent of lattice size but are dependent of temperature and the critical exponents.

On plotting the observed parameters for different lattice size, we get the corresponding critical exponent ratios.

## Numerical Analysis

### Temperature dependence of magnetization

We first studied the changes in the lattice (spin orientations at each lattice site) with temperature by plotting the ferromagnetic lattice for different temperatures. In figure 1, at low temperature  $T = 0.0001$  the yellow (spin up) and black (spin down) are in patches. This means the spin down and spin up particles were in groups of same spin orientation, clearly showing domain formation. Also we mostly observed yellow patches showing that most of the spins were aligned in one direction and had +1 value (note that even though the temperature is much lower than the critical temperature we still see black patches, i.e. all the spins are not aligned. This is probably because the figure is a plot of only the last configuration of the lattice and not an average configuration). But as the temperature was increased, for  $T = 2.0$ ,  $T = 10.0$ , we saw smaller but more patches implying smaller domain size. Also, the number of up spins had decreased and down spins had increased from before. Numerically this was because the system now had enough energy and by Metropolis algorithm, lattices with anti-parallel spins were accepted. Physically, there is a competition between independency (due to temperature) and interdependency (due to Exchange interaction between neighbors) of the spins. At high temperatures, thermal disorder wins over exchange interactions resulting in anti-parallel spin orientation [2]. At high temperatures  $T = 100$ , because all spin flips were accepted, we observed yellow and black dots which were more or less equal implying equal number of up and down spins. Again physically, since there was more thermal energy with the system, more anti-parallel spin orientations were possible.

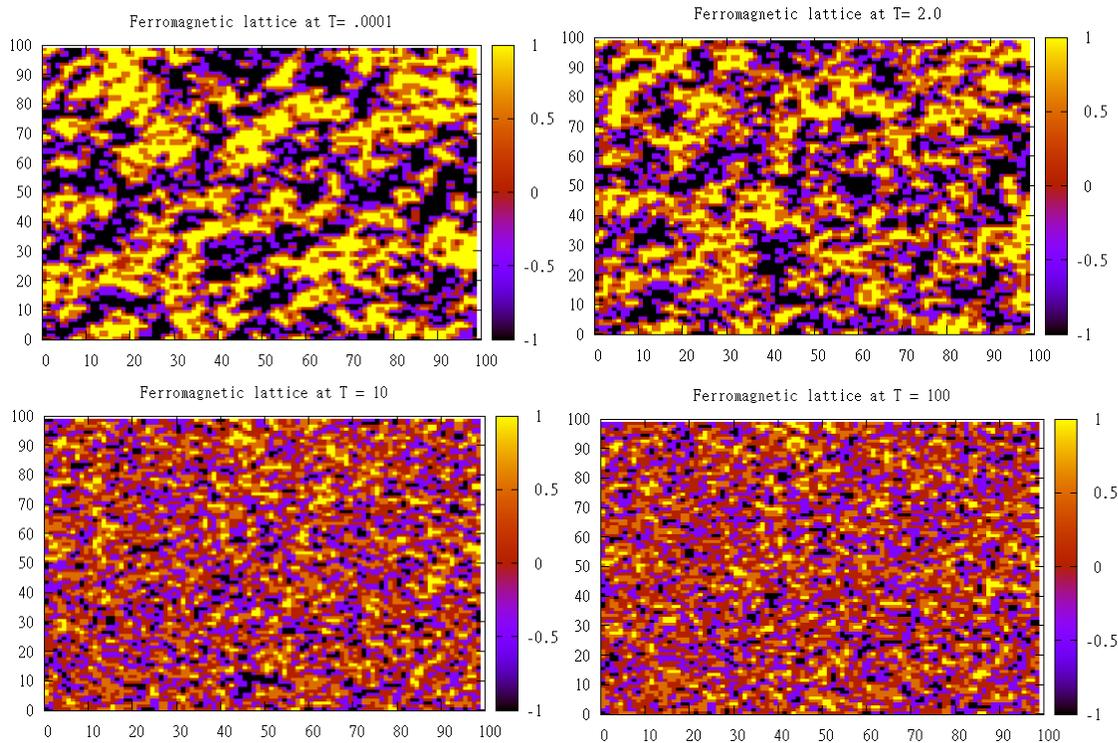


Figure 1: Ferromagnetic lattice at  $T = .0001, 2, 10$  and  $100$

Average magnetization,  $m$  is the order parameter for the Ising model. By studying the variation of magnetization with temperature, we can determine the critical temperature at which phase

transition is taking place. To study the temperature dependence of average magnetization,  $m$  of the Ising model we first found  $m$  using the following formula [4]:

$$m = \langle s_i \rangle \quad (\text{i.e the sum of all spins in the lattice})$$

and then studied the variation of absolute magnetization (abs  $m$ ) with temperature ( $T$ ). We found for a square lattice of length 100, at high temperatures around 10,000 the magnetization was  $0.0086 \approx 0$  since there were equal up and down spins. At temperatures around 10, absolute magnetization was 0.0098 still very close to zero (number of spins up and down were almost the same). But at low temperatures around 1, absolute magnetization became 1, since most spins were either aligned upwards or downwards. Figure 2 is a plot of abs  $m$  with  $T$  varying from 0.01 to 30.0 with steps of 0.1 also showing this variation. The temperature around which the magnetization started to reduce to zero, the critical temperature  $T_c$  was  $= 2.3$ . This is clearly seen in figure 3 where  $T$  varies from 1.0 to 3.0 with steps of .005 and 10,000 iteration steps.

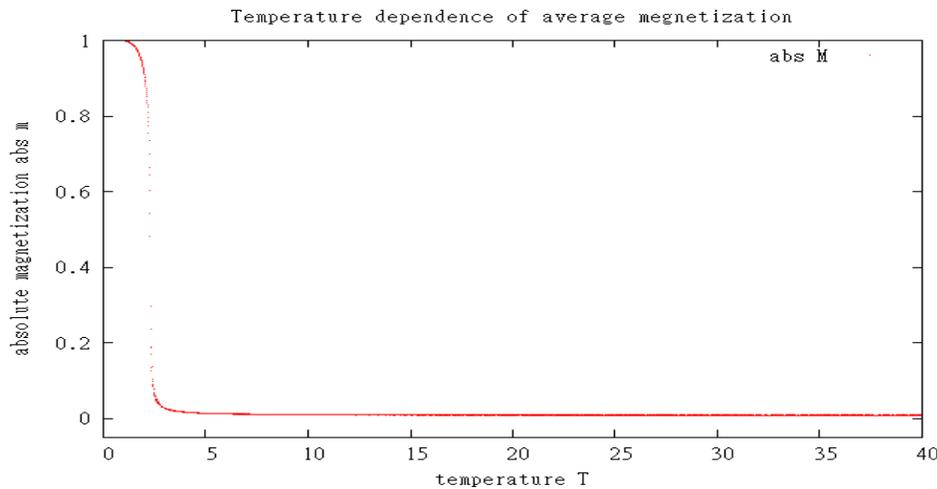


Figure 2: temperature dependence of average magnetization for lattice size 100

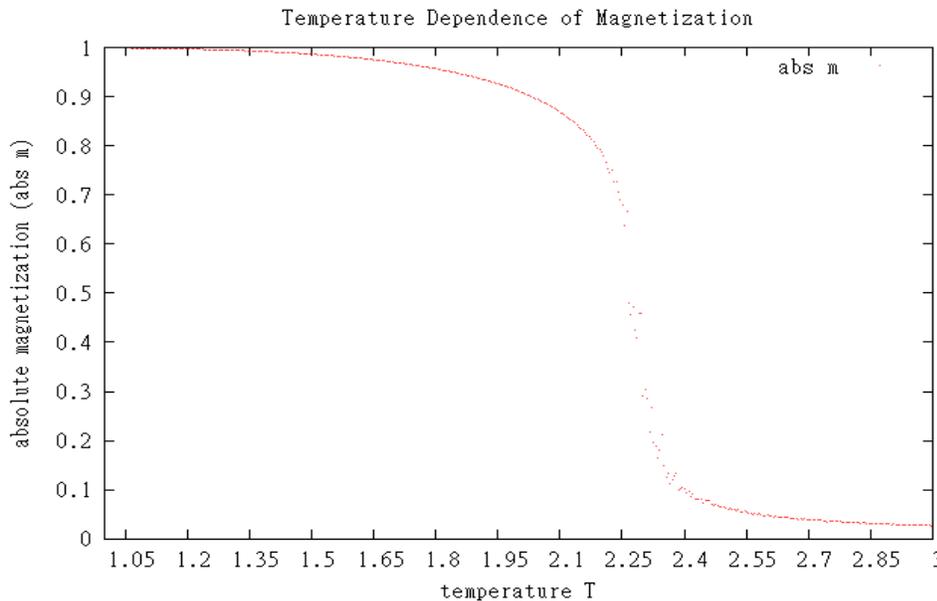


Figure 3: temperature dependence of absolute magnetization for temperature ranging from 1.0-3.0.  $T_c = 2.3$

Dependence of critical temperature on lattice size can be seen from figure 4. It plots absolute magnetization with temperature from 1.9 to 3.0 for different lattice size. For a smaller lattice, the system undergoes phase transition faster as compared to a larger lattice size. In figure 4 the critical temperature for lattice size 50×50 smaller than that for lattice size 150×150.

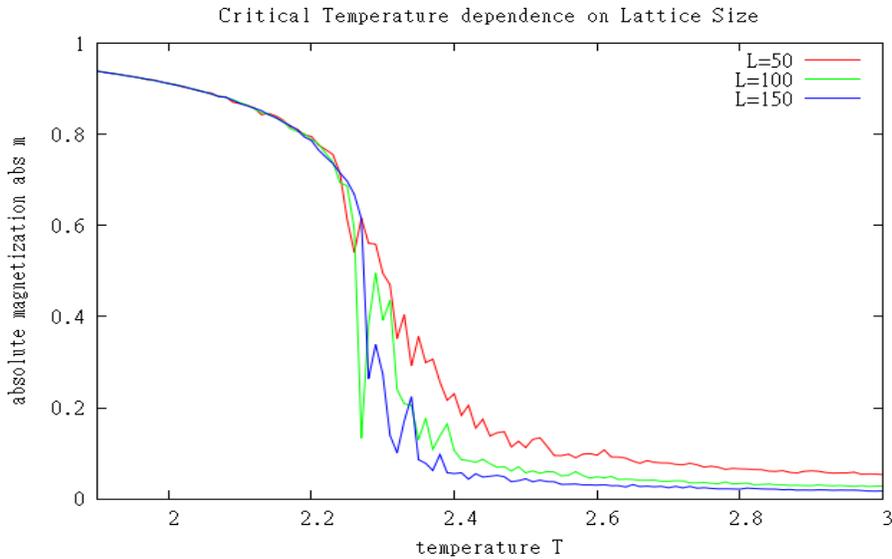


Figure 4: dependence of critical temperature on lattice size L= 50, 100 and 150

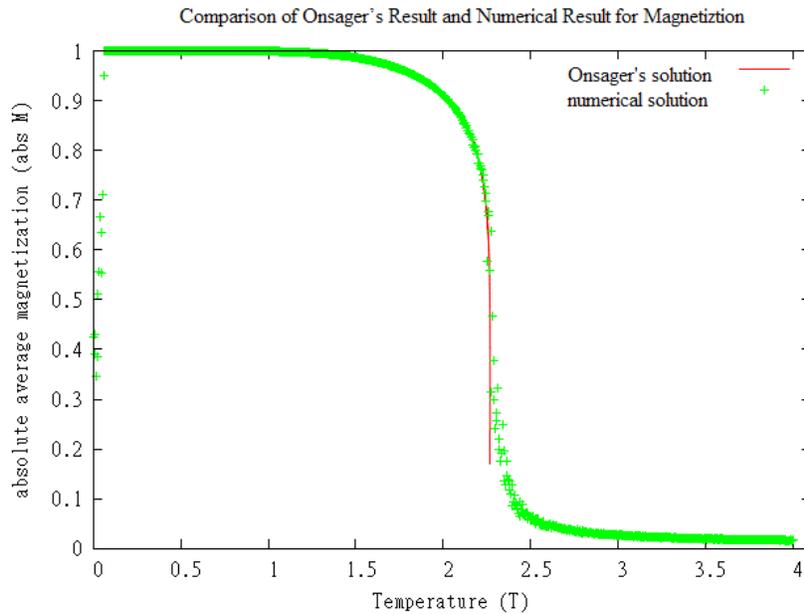


Figure 5: comparison between theoretical and experimental solution of critical temperature

In 1944, Lars Onsager solved the 2 dimensional Ising model with no applied external magnetic field and in 1949 he gave the solution for spontaneous magnetization as the following [5]:

$$M = \left\{ 1 - \left( \sinh \frac{2}{T} \right)^{-4} \right\}^{\frac{1}{8}}$$

The Comparison of the analytical solution of the magnetization given by Onsager with numerical solution (Monte Carlo technique) is shown in figure 5. The two curves are found to have the

same shape and a drop to zero magnetization at  $T = 2.26$  showing an agreement between the numerical and analytic calculations. The curve showing Onsager's solution doesn't touch zero in the plot. This is because the iteration steps were not small enough to coincide with the exact value of temperature for which Onsager's magnetization is zero. We used the maximum sample number, 1,000,000 in "Gnuplot 4.4" to attain this graph.

### Critical Exponents

The critical exponents are given by the following equation:

$$\begin{aligned}
 c &\propto (-\tau)^{-\alpha} \\
 m &\propto (-\tau)^\beta \\
 \chi &\propto (-\tau)^{-\gamma} \\
 \xi &\propto (-\tau)^{-\nu}
 \end{aligned}
 \quad \text{-equation (2)}$$

Where,  $c$  is the specific heat,  $m$  the spontaneous magnetization,  $\chi$  the susceptibility and  $\xi$  the correlation length. Doing finite size scaling (expressing the observables as a function of lattice size) we obtain equation (1). From this equation  $\beta/\nu$  could be found by plotting  $m$  vs.  $L$  on logarithmic axis. The slope of this plot gave  $\beta/\nu$ . Figure 6 is a plot of the root mean square value of average magnetization against different lattice size ranging from 10 to 120 with steps of 10 on logarithmic axis at  $T_c = 2.691$ . By mean square fit of the curve, the slope was found to be  $0.12545 \pm 0.02441$  which is  $\beta/\nu$ . The theoretical value for this ratio is 0.125.

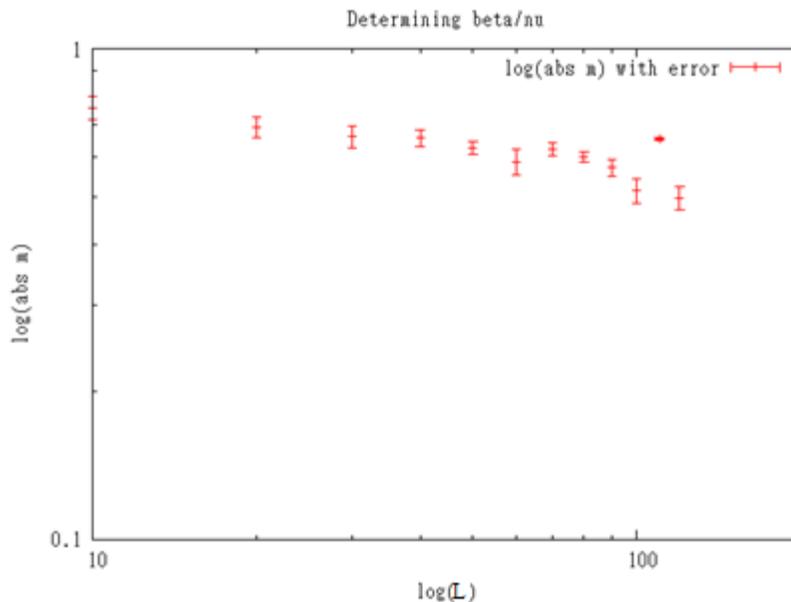


Figure 6: plot of absolute magnetization and temperature on logarithmic scale with error bars

### Autocorrelation function for Metropolis algorithm

The autocorrelation function for the Metropolis algorithm was studied and is shown in figure 7 for temperature  $T = .001$  and 10. It was found that at low temperatures  $T = .001$ , there was an exponential decay in correlation between the data after which it remained uncorrelated. This was because initially the distance between the data was not too big hence correlation between the

data points was possible. But with increase in time, the distance between data increased reducing the correlation. For higher temperature,  $T= 10$  only the first few data points were correlated and the rest uncorrelated with their autocorrelation function fluctuating randomly about zero.

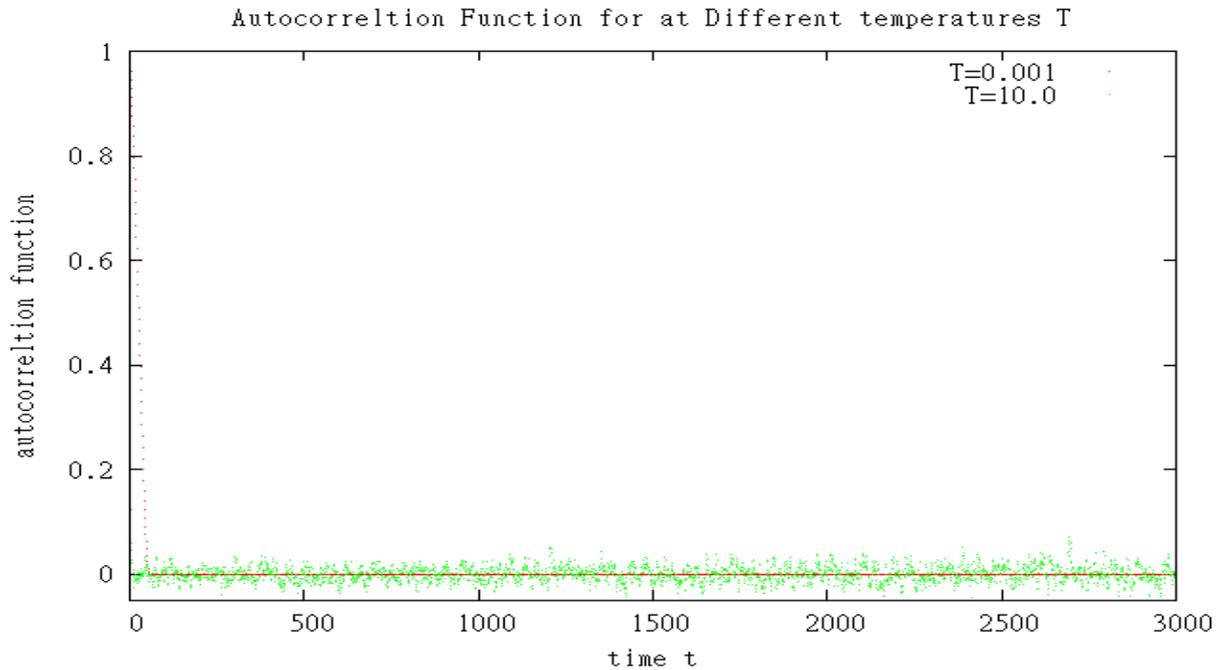


Figure 7: autocorrelation function for Metropolis algorithm at Temperature  $T= .001$  and  $10$ .

## **Summary**

Numerical and analytic relation for temperature dependence of spontaneous magnetization was found to be in agreement. Average magnetization was found to be 1 below critical temperature and approached 0 at temperatures higher than critical temperature. Critical temperature was found to be 2.3 and the ratio of  $\beta/\nu$  was found to be  $-0.12545 \pm 0.02441$ . Autocorrelation function for the Metropolis algorithm was found to be zero at high temperatures. For low temperatures it fell to zero and stayed there.

## **References**

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