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2D Ising Model and Ferromagnetic Phase Transition

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Abstract

Thermodynamic characteristics are studied for two dimensional Ising model. A 2D Monte Carlo code is developed to study the ferromagnetic properties and ferromagnetic phase transition. The code is written in FORTRAN. Thermodynamics parameters such as specific heat capacity and magnetic susceptibility are obtained out of the code for a range of temperatures. Ferromagnetic to paramagnetic phase transition (a second order phase transition) is observed in these thermodynamic quantities. Results are compared for various simulation box sizes.

INTRODUCTION

In ferromagnetic substances such as Iron, Nickel etc. there exists a spontaneous magnetization caused by the alignment of the magnetic spins in the same direction below a certain temperature, known as the Curie temperature [1]. It has been observed that if the spins are aligned in the same direction, their total energy decreases than if they are antiparallel [2]. This in turn gives the substance a tendency to keep the spins aligned. At a temperature more than the Curie temperature, average thermal energy of the spins is increased and the substance has approximately half of the spins aligned opposite to each other. This creates a net zero magnetization and the substance behaves as a paramagnetic material. At this instance, the material is said to have changed its phase from being ferromagnetic to paramagnetic. A ferromagnet has a non-zero magnetic field even when it has zero external magnetic field. On the other hand, a paramagnet has a magnetic moment only when it is in an external magnetic field. Magnetic moment per unit volume is known as the magnetization.

There has been a lot of research on this type of phase transition (ferromagnetic to paramagnetic) [2]–[5]. Although intuitively, the change of state of a matter is known as transition in phase, but, it must have a solid base of mathematics. This is however obtainable from the standard thermodynamic potentials. In the first order phase transition, thermodynamic quantities which

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are obtained from the first order derivatives of the free energy (F or G) show a discontinuity. On the other hand, in the second order phase transition, quantities obtained from the second order derivative of the above thermodynamic potentials show discontinuity.

Ferromagnetic to paramagnetic phase transition is a second order phase transition where the thermodynamic quantities namely the specific heat capacity and the magnetic susceptibility show a discontinuity at the critical temperature (T_c). They are indeed the fluctuations in the energy and the magnetization respectively. Mathematically, this is expressed as

$$C_v = \left(\frac{\partial E}{\partial T}\right)_B$$

And

$$\chi = \left(\frac{\partial M}{\partial B}\right)_T$$

In terms of fluctuations, the quantities are represented as follows.

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

And

$$\chi = \frac{< M^2 > - < M >^2}{k_B T}$$

E and M are the average energy and average magnetization per spin respectively. M is the order parameter which increases continuously from zero at the critical temperature. Another signature of the second order phase transition is the divergence of the susceptibility at the critical temperature. Since, $M = \chi H$, it tells how easily the spins respond to the external magnetic field.

In this article, the fluctuations in the energy and magnetization is calculated by using a suitable Monte Carlo scheme via Metropolis Algorithm and profiles of the average energy, magnetization, heat capacity and magnetic susceptibility are obtained for different simulation box sizes.

Numerical Execution

In order to execute the evolution of resulting thermodynamic profiles via Ising model, random spins are arranged over a 2D lattice. The Hamiltonian for the problem may be written as

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$$H = -J \sum_{<i,j>} S_i S_j - h \sum_{i=1,N} S_i$$

Here, the sum $< i, j >$ is over the nearest neighbor. J is a constant that specifies the strength of the interaction. Also, h is the external magnetic field. When $h > 0, S_i = +1$, otherwise, for $h < 0; S_i = -1$. This means spins want to align with the direction of h. If the applied magnetic field is zero, then the Hamiltonian is given by,

$$H = -J \sum_{<i,j>} S_i S_j$$

The algorithm for solving the problem is given below.

a. Arrange the atoms with random spins (or any specified spins such as +1 or -1) over a 2D lattice of definite size.
b. For any chosen random spin, calculate the energy of the lattice. Call it initial energy.
c. Give the chosen spin a trial flip and again calculate the energy of the lattice. Call it the final energy.
d. The difference in energy is $dE = E_{final} - E_{initial}$.
e. If $dE \leq 0$, accept the trial flip, as the system goes into a minimum energy configuration. Else, compute $u = \exp(-dE/kT)$ and compare this with a computer generated random number (r).
f. If $r < u$ accept the move, otherwise reject it.
g. Do it for all temperatures and find out the averaged thermodynamic quantities.

Results and Discussions

Fluctuations in the magnetization and the energy is shown in figure 1(a) and (b) respectively. The figure shows the results for various initialization of the spin orientations. It is seen that the final result is independent of the initial spin orientations. Energy is found to be the same in all the three cases. It is important to note that the spins are either aligned up or down. However, in an absolute sense this should not make any difference since, the direction or orientation is merely a visual choice.

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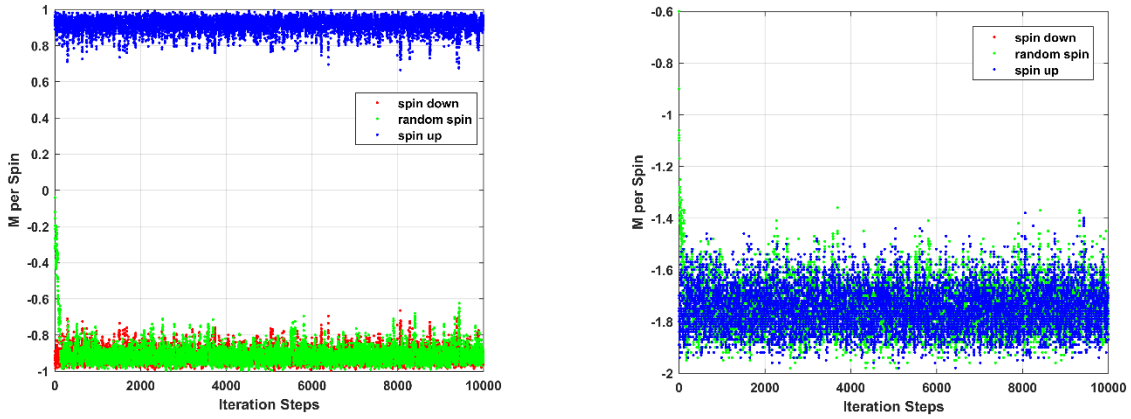

(a) (b)

Figure 1 (a), (b). Fluctuations in the magnetization per spin and energy per spin respectively.

The following figures (figure 2 and figure 3) show the profiles of average magnetization and energy, heat capacity and the susceptibility. The figures depict a phase transition at about a temperature of 2.269 (≈ 2.27). The black dotted line in each figure shows this point. Simulation box length considered for this evolution is L=20. This means, there are 20×20 spins randomly oriented initially. The evolutions are averaged over 100000 iteration steps.

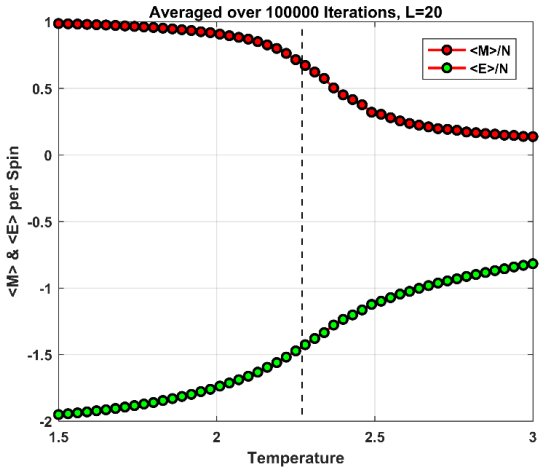

Figure 2. Average magnetization and energy per spin at box length L=20.

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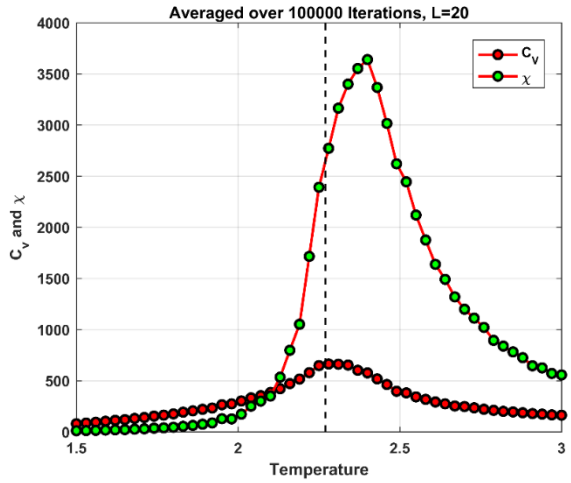

Figure 3. Average magnetization and energy per spin at box length L=20.

The ferromagnetic phase transition is a clearly indicated at the critical temperature $T_c = 2.27$. For the graph of heat capacity the indication is more prominent over the graph of susceptibility. In the following, a comparison of all of these parameters are shown for various box lengths. The figure depict the fact that with increasing box lengths, the variables are better averaged and the results are more accurate. The graph of average magnetization strongly establishes this fact.

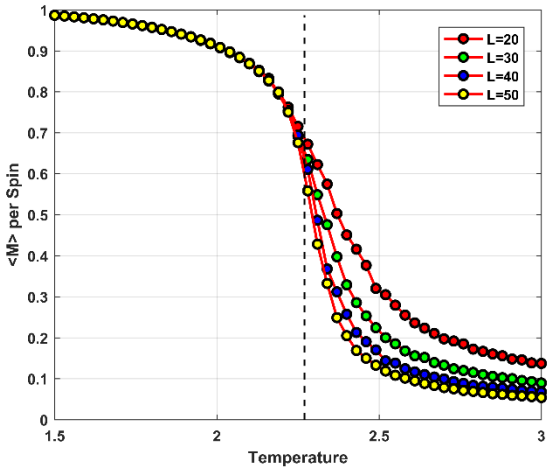

Figure 4. Average magnetization per spin for various box lengths.

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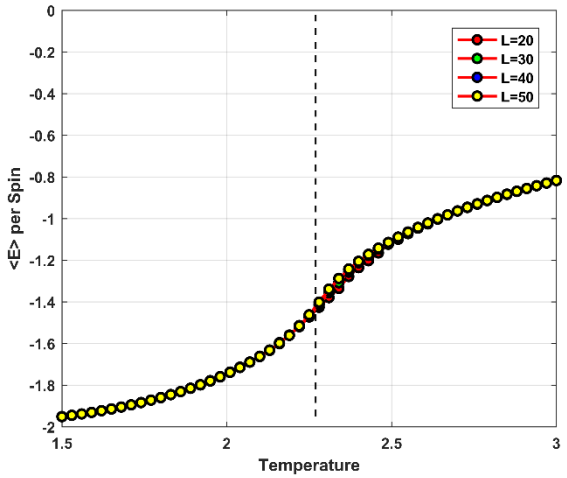

Figure 5. Average energy per spin for various box lengths.

It is imperative that the energy remains fixed (approximately) for all the box lengths. The fact is due to the canonical nature of the system. The system being canonical continuously exchanges energy with the environment or the heat bath. This in turn supplies any short fall of energy to the system, and the average energy remains fixed. Evolution of the Heat capacities and susceptibilities are shown in figure 6 and figure 7.

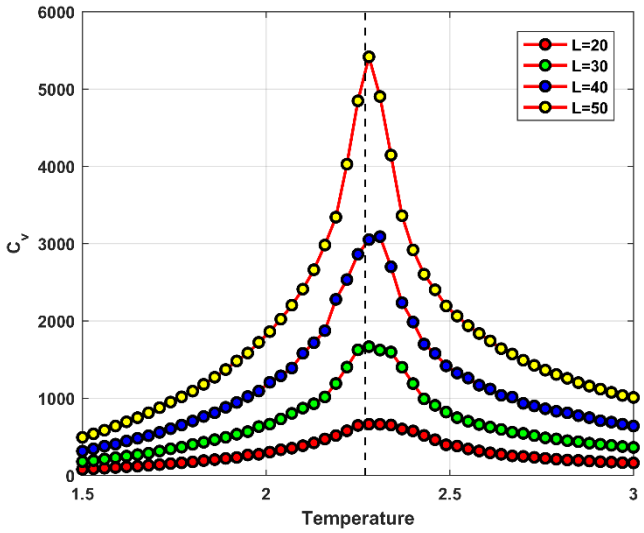

Figure 6. Heat capacities for various box lengths.

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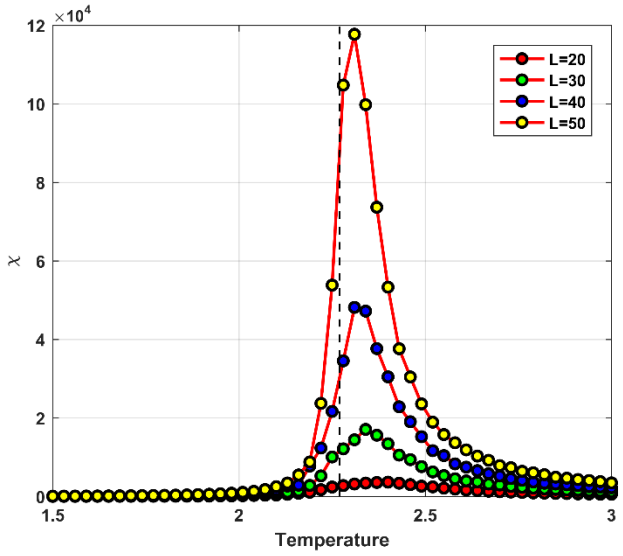

Figure 7. Susceptibilities at various box lengths

An interesting observation depicts the fact that the peak of the susceptibility approaches near the critical temperature for higher box lengths. The magnitudes of both heat capacity and susceptibility increases with the increase in box lengths. Here, it is worth noting that the graphs for higher box lengths are averaged over longer iteration steps.

The code employed for obtaining the results is a serial code. For a computational work it is important to mention the time of computation. In the following, Table-1 compares the simulation times for various box sizes. The comparison is for 110000 iteration steps with an increase in temperature steps equating 3 (T=1.5, 3). Data is allowed to write at each temperature step. For the lattice size 50×50, in order to achieve smooth profile iteration steps were increased up to 5×10^5 in the graphs, but kept 110000 in the table-1.

Table: 1 Simulation time for various box sizes (serial run)

Sl. No.	**Box Size**	**Simulation Time (sec)**
1.	20×20	305.564
2.	30×30	688.504
3.	40×40	1214.840
4.	50×50	1891.400

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The computational time evolution with box sizes is plotted in figure 8. The figure depicts almost an exponential rise in the computational time of the simulation. This insists the use of parallel computing while computing over larger box sizes. However that is beyond the scope of this paper.

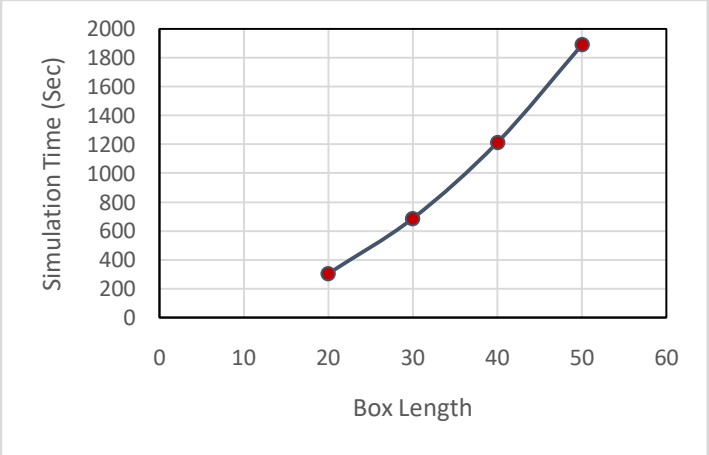

Figure 8. Computational Time for serial run in different box lengths.

Conclusions

Ferromagnetic phase transition is studied in Ising model via Monte Carlo Metropolis algorithm. The model is solved for a 2D square lattice with randomly oriented spins. The transition being second order in nature, plots for the heat capacities and susceptibilities are obtained. Both of these parameters show a kink at the critical temperature. The computational variables are compared for various box lengths and it has been observed that increasing the box lengths increases the exactness of the results. In other words, the results become more appropriate for higher box lengths. It should be noted that increasing the box lengths also increases the computational time. This however can be solved by doing a suitable parallelization of the code.

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