Monte-Carlo Simulation of Phase Transition in 2D and 3D Ising Model

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Abstract

In this work, Markov Chain-Monte Carlo technique was used to study the phase transition in two and three dimensional Ising Model in a square and cubic lattice. The study of temperature dependence of average magnetization and specific heat in different magnetic fields has been carried out in 3x3 and 3x3x3 lattice with periodic boundary. Critical temperature points $k_B T_c/J$ for 2D and 3D IM has been observed at around 2.2 and 4.3 respectively at zero field. Our work satisfies Onsager's critical value in 2D IM. The simulation suggests bifurcation in average magnetization below critical temperature T_c. Temperature plays role of increasing randomness of spins. We found IM in small lattice size still retains interesting features like spontaneous magnetization and symmetry breaking below T_c at $B = 0$. At non-zero field, the likelihood of spins to prefer certain alignment depends on the direction of external field and magnitude of magnetization depends on magnitude of field $\pm B$.

Keywords: Critical temperature; Markov-chain; Phase transition; Spontaneous magnetization; Symmetry breaking.

1. Introduction

Ising Model (IM) was a problem in 1D given by Whilhelm Lenz to his student Ernst Ising for his PhD thesis[1], which was published in 1925. It was a simple statistical mechanical model to study phase transition in ferromagnets with one-dimensional chain of spins which are represented by either +1 or -1. Later, in 1943 Onsager[2] solved the two-dimensional IM in zero field, by using theoretical technique of transfer matrix and group theory which explains the transition of magnetic properties of ferromagnet into paramagnet above critical temperature. Even nearly after a century, the model remains one among the few analytically solved statistical problem with it's applications in wide disciplines of science. The toroidal topology of 2D Ising Model with periodic boundary is shown in Fig. 1 in which the spins are supposed to be situated in the vertices of the toroid. The red and blue arrows in loops represent periodic boundary condition (PBC). The use of PBC is a heuristic approach towards making lattice of infinite size.

Phase transition is characterised by abrupt change in a physical quantity with small variation of parameter. Ising found no phase transition in one-dimensional IM and concluded the similar expectation for higher dimensions. Onsager found there exists phase transition in two dimensional model. Exact solution of higher dimensional IM has remained intractable problem for both physicists and mathematicians, although various approximation works have been done. In order to address this issue, a powerful algorithm has been developed, called Markov-Chain Monte Carlo simulation, whose results elegantly match with theory.

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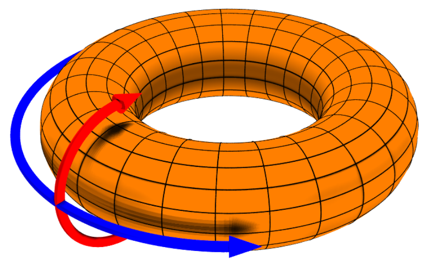

Fig. 1. Toroidal topology of 2D Ising Model[3], arrows showing PBC.

Ising model is a famous toy model originally developed to explain the phase transition in ferromagnets whose two dimensional analytic treatment is still under development. It has been subject of successive historical development following the proof of Peierls[4], who verified the existence of phase transition in 2D. This work was followed by Kramers and Wannier[5] to predict the critical temperature. Onsager computed free energy and average magnetization of 2D IM at zero field and found the critical point[2] to be $k_B T_c / J = 2.269185$. There are thousands of paper on Ising Model(IM) on the recent developments. The summary of findings of all historical progresses in IM can be found in textbook of McCoy and Wu[6].

Varieties of simulation techniques have been developed to model physical processes and run it in computers. Metropolis algorithm[7] is one standard method of drawing sample configuration of IM for particular temperature from random configuration of phase space. K. Binder[8] has discussed application of Monte-Carlo method to problems of statistical physics. The method makes use of Markov Chains to generate desired sample. The algorithm makes decision to accept or reject changes in spins based on a transition probability for the markov chain such that it has a Boltzmann distribution.

1.1. Hamiltonian of IM

In this section, we will introduce the hamiltonian of Ising Model which will be used to compute energy and specific heat in our simulation work. It is also a pre-requisite to formulate the partition function, which can be used to obtain any of the thermodynamic quantities theoretically. The critical point of 2D IM so obtained at zero field has been compared with results of our simulation. Hamiltonian of IM (H), in general depends on external magnetic field B and interaction strength J, where μ is moment which represents the inherent strength of spins.

$$H = -\mu B \sum_{i} s_i - J \sum_{i,j} s_i s_j \tag{1}$$

where i in first term runs over all spins.
i, j in second term runs over non redundant pair of neighboring spins.
The first term in Equation 1 addresses the self energy of spins in presence of external field B. For B>0, the first term is negative for +1 spin and positive for -1 spin. This shows up spin i.e. +1 is biased for B>0, as it lowers the hamiltonian. Similarly, for B<0, down spin i.e. -1 is biased. Second term accounts for interaction between neighbors. J>0 ; i.e +ve J for ferromagnetic substance, assuring same adjacent spins lowers Hamiltonian of system. J<0 for anti-ferromagnetic substance, favoring the alignment of opposite spins in neighbourhood.

Although analytical solution of 2D Ising Model at zero field has been computed, the exact solution of

3D and higher dimensional IM does not exist till date and hence, MCMC simulation is considered a powerful technique to study phase transition of $D \geq 3$ dimensional IM model. Firstly, we will introduce the preliminaries of statistical mechanics that are essential before proceeding to 2D IM and simulations. Our analysis of phase transition in 2D IM requires concepts of partition function, Boltzmann probability and relative probability which are discussed in the sections 1.2.

1.2. Partition Function, Boltzmann Probability, and Relative Probability

Partition function is a functional in statistical mechanics on which certain operations are done to get the value of physical observable. Partition function contains all the information needed to recover the macroscopic properties of a thermodynamic system with fixed number of particles immersed in a heatbath[9,10]. We will use the expression of partition function without details of formulation of canonical ensemble.

$$\mathcal{Z} = \sum_i e^{-\beta H_i} \; ; \; \beta = \frac{1}{k_B T} \tag{2}$$

where,
k_B=Boltzmann Constant
T=Absolute Temperature
i=Possible Spin Configuration
H_i=Hamiltonian of state i

The Boltzmann probalility which is the probabilty of i^{th} spin configuration is denoted by p_i and explicitly depends on Hamiltonian H_i and inverse temperature β .

$$p_i = \frac{e^{-\beta H_i}}{\sum_i e^{-\beta H_i}} = \frac{e^{-\beta H_i}}{\mathcal{Z}} \tag{3}$$

Partition function, $\mathcal{Z}$ appears as a normalizing factor to ensure probability sum to one in Boltzmann probability.

Relative probability is used to decide whether to accept or reject the sample of spin configuration which will be used for simulation in our work. It is the ratio of Boltzmann probability of final state p_{final} to initial state $p_{initial}$ in a transition.

$$R = \frac{p_{final}}{p_{initial}} = \frac{e^{-\beta H_{final}}}{e^{-\beta H_{initial}}} = e^{-\beta \Delta H} \tag{4}$$

where,
$\Delta H = H_{final} - H_{initial} =$ Change in Hamiltonian

2. Methodology

2.1. Theory

In our work, we compute the three quantities: magnetization, specific heat and energy of selected samples for simulation. We use magnetization (M) to find the average of spins of Ising System which ranges from -1 to +1. The value of magnetization is close to zero when spins are randomly arranged. Higher number of +1 spins compared to -1 spins shift M above zero whereas higher number -1 spins compared to +1 spins shift M below zero. The middle term in Equation 5 is used to compute the magnetization of the spin configuration in our work. The last term in Equation 5 is used for theoretical calculation of magnetization.

$$M(N,T,\mu B) = \left\langle \sum_{i=1}^{N} s_i \right\rangle = k_B T \frac{1}{\mu \mathcal{Z}} \frac{\partial}{\partial B} \mathcal{Z} \tag{5}$$

Onsager performed the theoretical calculation of magnetization in Ising Model. We compare this theoretical value of magnetization with the value of magnetization obtained through simulation technique.

Energy is the average hamiltonian of Ising system and defined by equation (6). The middle term in Equation 6 has been used to calculate the energy of spin configuration in our work. Energy of Ising system is governed by two terms. The first term with external field B is self energy term of spin when the spin experiences field B. The later term which has coupler J incorporates interaction energy due to nearest neighboring spins.

$$E = \left\langle -\mu B \sum_i s_i - J \sum_{i,j} s_i s_j \right\rangle = -\frac{\partial \; ln\, \mathcal{Z}}{\partial \beta} = -\frac{1}{\mathcal{Z}} \frac{\partial \, \mathcal{Z}}{\partial \beta} \tag{6}$$

Specific heat C_v is generally given by change in energy with change temperature.

$$C_v = \frac{\partial E}{\partial T} \tag{7}$$

According to the fluctuation dissipation theorem, specific heat C_v can be expressed as,

$$C_v = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T} \tag{8}$$

The behaviour of phase transition can be explained by studying the variation of specific heat with temperature. In our work, standard deviation of energy of thermalized samples of spin configuration has been used to calculate specific heat at particular temperature. This gives the fluctuation in energy of thermalized samples at corresponding temperature regimes.

Onsager's Results:
We will compare the phase transition as predicted theoretically by Onsager[2] with our simulation work. Onsager derived the expression of magnetization in 2D IM in zero field and found the value of critical point to be 2.269185 J. The magnetization at different ranges of temperature is given by,

$$M(T) = \begin{cases} \frac{(1+z^2)^{\frac{1}{4}}(1-6z^2+z^4)}{\sqrt{1-z^2}} & \text{if } T < T_c \\ \\ 0 & \text{if } T > T_c \end{cases} \tag{9}$$

where, $z = e^{\frac{-2J}{k_B T}}$
The critical temperature T_c from theoretical approach given by Onsager can be obtained from Equation 10,

$$k_B T_c = 2.269185 J \tag{10}$$

2.2. Simulation Technique

2.2.1. Markov Chain Monte Carlo Algorithm

Monte-Carlo method relies on use of random numbers and helps in probabilistic description of a problem. MCMC which is a sampling technique which leads us to desired phase space configuration corresponding

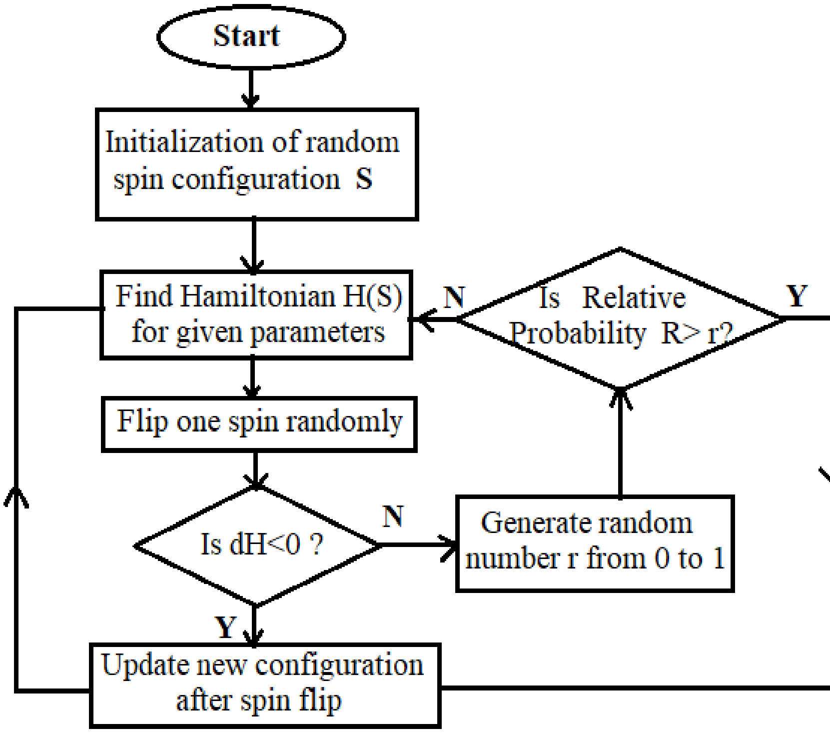

Fig. 2. MCMC thermalization algorithm

to peak of distribution for a specific temperature. We will start with a random configuration and let the system evolve to a state of uniform energy that maximizes entropy. This process is called thermalization. During the thermalization process, the transition takes place through a sequence of configuration states, and it produces a Markov Chain. The heart of this algorithm is in generation of a random spin configuration with Boltzmann probability by making decisions to accept or reject random spin flips[11].

We will take a finite size of square or cubic lattice with 3x3 or 3x3x3 spins in a periodic boundary condition. We can either start with all spins down or all spins up or arbitrary spins. Hamiltonian and Magnetization of a spin configuration in a lattice is calculated. One of the spin is randomly flipped and decision for accepting or rejecting the new spin configuration is performed based on Boltzmann Probability values of configuration. When the sequence of accepted configurations attain stable values of hamiltonian, the samples are said to be thermalized. We will retain history of Hamiltonian and Magnetization during nrun thermalizations which is done at constant temperature. Average of spin, standard deviation of Hamiltonian History and average of Hamiltonian History; only after 2000^{th} thermalizations will be taken for computation of Average Magnetization, Specific Heat and Energy. Then after, we will increase T and repeat the procedure. We have set the values of parameters K_b, J and μ equal to 1 throughout simulation.

There are some limitations of MCMC method. The computers generate pseudo-random numbers and simulation lacks perfect randomness. It is necessary to take finite lattice size for computation and simulate the system for finite observation time. Statistical Errors arise due to such limitations.

Markov Chain Monte-Carlo algorithm is implemented in following steps:

1. Starting with arbitary spin configuration $U_k = \{s_1, s_2, ..., s_N\}$

2. Generating a trial configuration U_{k+1} by picking a random spin s_i and flipping it $s_i = -s_i$

3. Calculating Hamiltonian of trial configuration H_{trial}.
   If $H_{trial} \leq H_{S_k}$, accepting trial by setting $U_{k+1} = U_{trial}$
   If $H_{trial} > H_{S_k}$, accepting with relative probability $R = e^{-\Delta E/k_B T}$

4. Choosing uniform random number $0 \leq r_i \leq 1$
   Accepting if $R \geq r_i$ by setting $U_{k+1} = U_{trial}$
   Rejecting if $R < r_i$ i.e. $\mathrm{U}_{k+1} = U_k$

3. Results and Discussion

3.1. Simulation in 2D IM

Although the lattice size is very small (3x3), it has been found to retain features of phase transition. Thermalization of Ising Model in 2D for higher lattice size of 15x15 and 20x20 in Figs. 3 and 4 shows that magnetization has been settled after certain number of nruns.

3.1.1. Thermalization in 2D IM

Thermalization is transition of arbitary spin configuration towards state with uniform energy for a particular temperature. We initialize the thermalization algorithm with two types of configuration, first cold start (all spins up) and then hot start (random spin configuration), and plot the evolution of magnetization at different runs through the markov-chain. Only the thermalized samples will be considered for computation of thermodynamic quantities of interest.

Fig. 3(a) shows the thermalization for two dimensional IM with lattice size of 20X20 and 15X15 respectively at temperature T=6 J/K_B and field B=0. Black curve represents thermalization with cold start configuration whereas green curve represents thermalization with hot start configuration. The evolution of markov chain in this case settles down to zero average magnetization as shown in Figure 3(a). Figure 4 shows the thermalization at temperature T=5 J/K_B and field B=1 for two dimensional lattice with lattice size of 20X20 and 15X15 respectively. In this case, the sample thermalizes at about magnetization close to 0.5. We will plot average of magnetization of such thermalized sample for discrete temperature points in plot of magnetization as a function of temperature.

We can observe the magnetization settles down after about 1000^{th} run of thermalization. To be sure that the sample we are taking represents thermalized sample, we take samples 2000^{th} nrun onwards for computation.

3.1.2. Findings of PhT in 2D IM

Bifurcation in magnetization below T_c shows symmetry breaking in zero field at low temperature region. Spontaneous magnetization has been observed below T_c in absence of external field, with equal tendency to align in either +1 or -1 alignment of spins in 2D IM model. Average magnetization shows a reflection symmetry along B=0 for curves of $\pm B$. A hump has been observed in specific heat of 2D IM near critical temperature for every field. At external magnetic field B=0, logarithmic divergence at critical

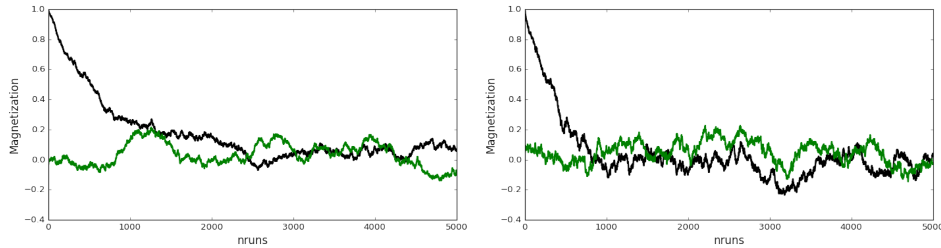

Fig. 3. In 2D IM at B=0, the thermalization at T= 6 J/K_B (a) for lattice size L=20 and (b) for lattice size L=15 respectively.

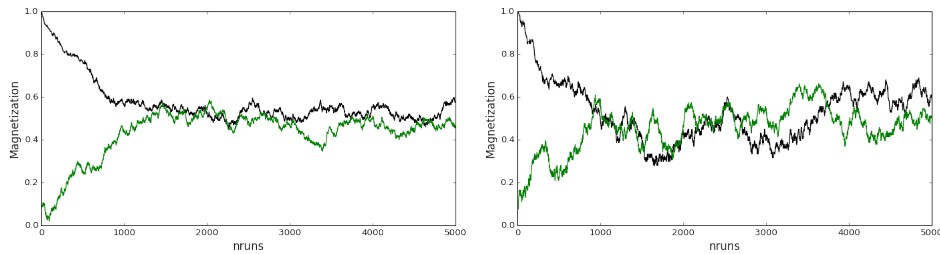

Fig. 4. In 2D IM at B=1, the thermalization at T= 5 J/K_B (a) for lattice size L=20 and (b) for lattice size L=15 respectively.

temperature has been observed where specific heat fails to be analytic function of temperature, which is in agreement with theoretical analysis of B. McCoy and T. Wu[6] (see Fig. 5(b)). In Fig. 5(a), the vertical red dotted line represents the critical temperature $T_c = 2.26\ J/K_B$ and red scatter plot below $T_c = 2.26$ represent magnetization obtained through Onsager's theoretical technique. Critical temperature obtained from observation of simulation around T_c=2.2 J/K_B has been found consistent with Onsager's critical temperature of $T_c = 2.26\ J/K_B$. The hump of specific heat in Fig. 5(b) has been observed behind the the critical temperature represented by vertical red dashed line.

3.2. Simulation in 3D IM

27 spins were put in a 3x3x3 lattice with periodic boundary and thermalization was initiated. The Fig. 7 shows that magnetization has been settled after certain nruns in thermalization of 3D Ising Model.

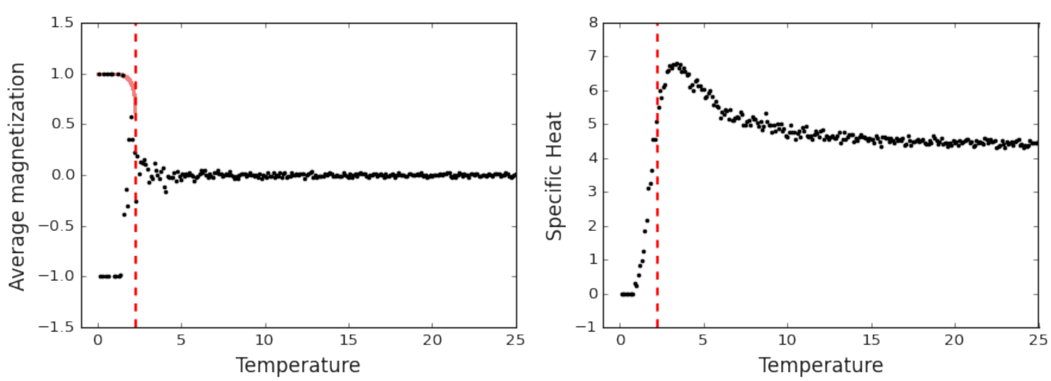

Fig. 5. In 2D IM, at B=0 (a) the temperature dependence of average magnetization and (b) the temperature dependence of specific heat.

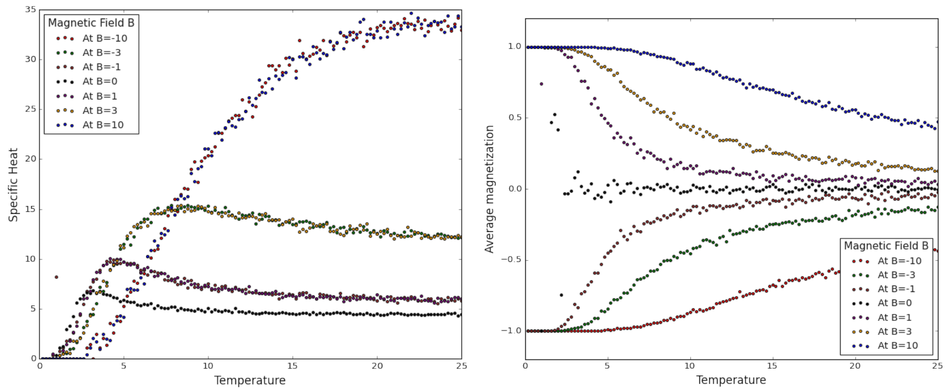

Fig. 6. (a) The temperature dependence of average magnetization and (b) the temperature dependence of specific heat in 2D IM at different fields.

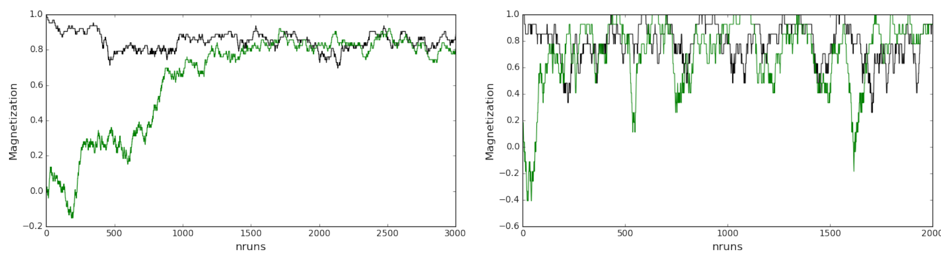

Fig. 7. Thermalization at T=5 J/K_B, B=1 for lattice size L=5 and L=3 respectively in 3D IM.

3.2.1. Thermalizaton in 3D IM

Like in 2D simulation, we initialize the thermalization algorithm with cold start and hot start, and plot the evolution of magnetization at different runs through the markov chain. Only the thermalized samples will be considered for computation of thermodynamic quantities of interest.

The Fig. 7 shows the thermalization for three dimensional lattice with lattice size of 5x5x5 and 3x3x3 respectively at temperature T=5 J/K_B and field B=1. Black curve represents initialization with cold spin configuration whereas green represents initialization with hot start configuration. We can observe the magnetization settles down at about 1500^{th} thermalization in L=5 and 200^{th} thermalization in L=3. To be sure that the sample we are taking represents thermalized sample, we have taken samples 2000^{th} nrun onwards for computation.

3.2.2. Findings of PhT in 3D IM

The simulation suggests critical temperature around T_c=4.3 J/K_B (as shown in Fig. 8). Simulation suggests specific heat increases on increasing temperature below T_c, falls down right after critical point and then attains nearly constant value at B=0 as observed in Fig. 8 (b). A prominent hump has been observed in specific heat of 3D IM showing qualitatively similar behavior as 2D. The hump at zero field represents the critical temperature below which symmetry breaking has been observed in magnetization. Spontaneous magnetization has been observed below T_c in absence of external field, with equal tendency to align in either +1 or -1 alignment. Average magnetization at non zero field shows a reflection symmetry along line at B = 0 for curves of $\pm B$ like in 2D.

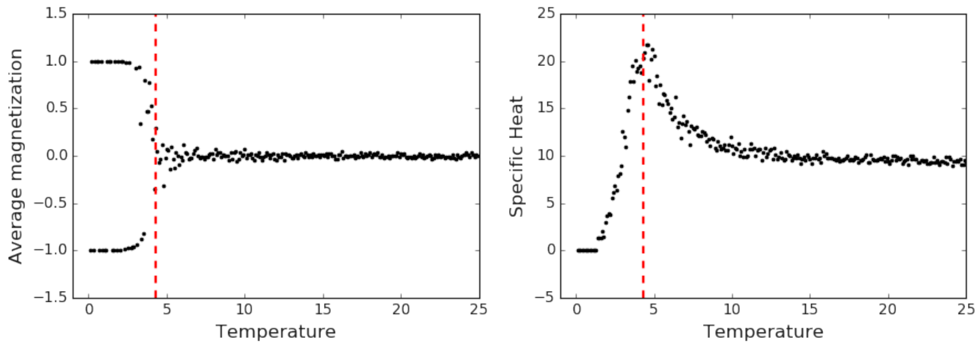

Fig. 8. In 3D IM, at B=0 (a) the temperature dependence of average magnetization and (b) the temperature dependence of specific heat.

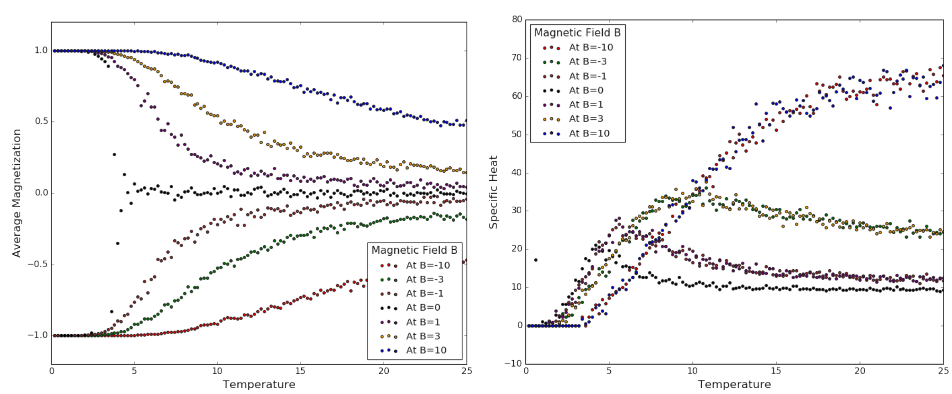

Fig. 9. (a) The temperature dependence of average magnetization and (b) the temperature dependence of specific heat in 3D IM at different fields.

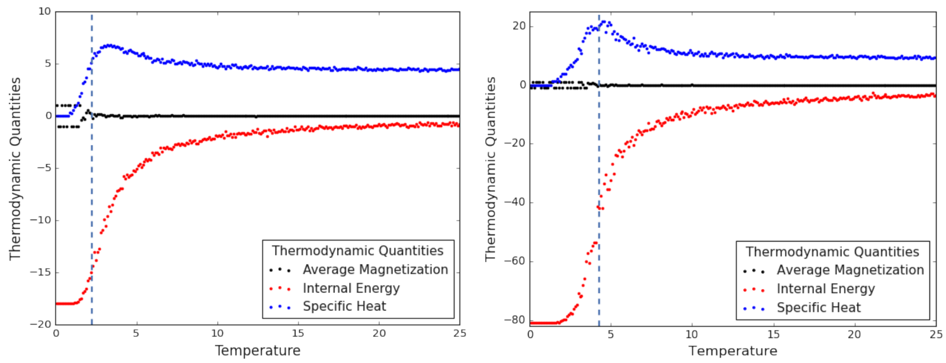

Fig. 10. The temperature dependence of average magnetization (black), specific heat (blue) and energy (red) at zero field for 2D and 3D IM. (a) the vertical blue dashed line represents Onsager's critical point T_c = 2.269 $k_B T_c/J$ in 2D and (b) the blue vertical dashed line represents critical point obtained from simulation in 3D IM.

3.3. Comparison of PhT in 2D and 3D IM

The 3D model shows qualitatively same results as 2D model. We found IM in small lattice size of 3x3 and 3x3x3 still retains features of phase transition. Our critical point satisfies Onsager's critical value in 2D IM at zero field. The simulation suggests bifurcation in average magnetization below critical temperature T_c in both 2D and 3D IM. This means there are two equally likely states of spin configuration below critical temperature. Increasing temperature has been found to contribute towards increasing randomness of spins. This conclusion could be drawn from inclination of magnetization towards zero at higher temperature. It has been found that IM exhibits interesting properties like spontaneous magnetization and symmetry breaking below T_c at $B = 0$. The specific heat, which is the measure of energy fluctuation at certain temperature has been found to attain hump at the critical region. The scatter points of specific heat C_v are found to be coincident for either of external fields $\pm B$. Evolution of specific heat starts from zero at regime below T_c grows to peak value at critical point. Specific heat lowers above critical point T_c and attains a stable value as shown in blue scatter plot of Fig 10. The fluctuation of energy of thermalized samples has increased on increasing magnitude of external field below critical temperature.

Conclusion

In simulation of phase transition in 2D and 3D Ising system, the bifurcation of magnetization below T_c at zero field shows that there are two equally possible states of configuration of spins (either all spins +1 or or all spins -1) in region below critical temperature represented by red vertical dashed line. Above critical temperature, either of the states collapse to a single state with random spin configuration in a system. In such a random spin configuration, the average magnetization is zero due to nearly equal number of +1 and -1 spins in Ising system. This physically signifies the loss in magnetic property above critical temperature. This bifurcation of magnetization shows that PhT in Ising model in 2D and higher dimensions exhibit property of symmetry breaking. As the magnetization is significant in absence of external field below T_c, this phenomena has been attributed as spontaneous magnetization.

The plot of specific heat C_v as a function of temperature exhibits characterstic hump near critical region. This shows that the fluctuation of energy in Ising system is maximum in region of phase transition. Our simulation observed in small finite lattice of 2D has shown hump behind the theoretical critical point obtained by Onsager. At non-zero field, the likelihood of spins to prefer certain alignment depends on the direction of external field and magnitude of magnetization depends on magnitude of field $\pm B$. Temperature plays role of increasing randomness of spins. The comparison of phT in 2D and 3D IM shows that the value of critical temperature in 3D Ising model is approximately twice the value of critical temperature in 2D Ising Model.

On increasing the value of external field, the hump of specific heat has shifted towards higher temperature.At extremely high external field, it has been observed that the value of specific heat C_v, which represents fluctuation in energy is found to be zero, which implies that energy of thermalized samples remains constant. This occurs because all spins of Ising system align along the direction of external field and hamiltonian doesn't vary. This phenomenon is prominent both in 2D and 3D.

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