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 (IM) 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 the 3x3 and 3x3x3 lattice with periodic boundary. Critical temperature point $\frac{k_B T_c}{J}$ for 2D and 3D Ising Model 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 the role of increasing randomness of spins. We found that Ising Model in small lattice size still retains interesting features like spontaneous magnetization and symmetry breaking below T_c at $B = 0$. At a non-zero field, the likelihood of spins to prefer certain alignment depends on the direction of the external field and magnitude of magnetization depends on magnitude of field $\pm B$. Specific heat C_v, which gives us fluctuation of energy at particular temperature, has been found to attain maximum value at critical regions.

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

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 (PhT) in ferromagnets with a 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 the 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 problems with its applications in wide disciplines of science. The toroidal topology of the 2D Ising Model with periodic boundary is shown in Figure 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 conditions (PBC). The use of PBC is a heuristic approach towards making a lattice of infinite size.

Phase transition is characterized 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. Later, Onsager[2] found there exists phase transition in a

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two-dimensional model. Exact solution of higher dimensional 'IM' has remained an 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.

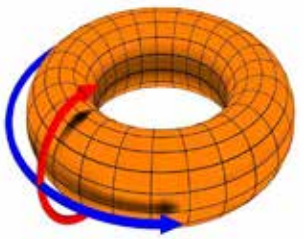

Figure 1: Toroidal topology of 2D Ising Model[3], arrows showing PBC.

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 solved the partition function problem and criticality[2] of 2D IM, but did not explicitly mention the critical value. Huang[6] calculated the critical point of 2D IM to be $\frac{k_B T_c}{J}$ = 2.269185. There are thousands of papers on 'IM' on the recent developments. The summary of findings of all historical progress in 'IM' can be found in the textbook of McCoy and Wu[7].

Varieties of simulation techniques have been developed to model physical processes and run it in computers. Metropolis algorithm[8] is one standard method of drawing sample configuration of IM for particular temperature from random configuration of phase space. K. Binder[9] has discussed application of Monte Carlo method to problems of statistical physics. The method makes use of Markov Chains to generate the desired sample. The algorithm makes a decision to accept or reject changes in spins based on a transition probability for the Markov chain such that it has a Boltzmann distribution.

Hamiltonian of IM

In this section, we will introduce the Hamiltonian of IM which will be used to compute energy and specific heat in our simulation work. It is also a prerequisite 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. The Hamiltonian of IM (H), in general, depends on external magnetic field B and interaction strength J, where μ is the moment which represents the inherent strength of spins.

$$H = -\mu B \sum_i s_i - J\sum_{i,j} s_i s_j \quad \ldots\ldots \quad (1)$$

Where i in first term runs over all spins and i,j in the second term run over non redundant pairs 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 that +1 spin is biased for $B > 0$, as it lowers the Hamiltonian. Similarly, for $B < 0$, -1 spin is biased. Second term accounts for interaction between neighbors. $J > 0$; i.e. +ve J for ferromagnetic substance, assuring the same adjacent spins lowers the Hamiltonian of the system. $J < 0$ for anti-ferromagnetic substance, favoring the alignment of opposite spins in the 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, Markov-Chain Monte Carlo (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.

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 a fixed number of particles immersed in a heatbath[10,11]. We will use the expression of partition function without details of formulation of canonical ensemble.

$$\mathrm{Z} = \sum_i e^{-\beta H_i} \text{ and } \beta = \frac{1}{k_B T} \quad \ldots\ldots \quad (2)$$

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

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

$$p_i = \frac{e^{-\beta H_i}}{\sum_i \beta H_i} = \frac{e^{-\beta H_i}}{\mathrm{z}} \quad \ldots\ldots \quad (3)$$

In Boltzmann probability, partition function z appears as a normalizing factor to ensure probability sum to one. 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.

$$R = \frac{P_{final}}{P_{initial}} = \frac{e^{-\beta H_{final}}}{e^{-\beta H_{initial}}} = e^{-\beta \Delta H} \quad \ldots (4)$$

Where $\Delta H = H_{final} - H_{initial}$ = change in Hamiltonian.

Methodology

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 the Ising System which ranges from -1 to +1. The value of magnetization is close to zero when spins are randomly arranged. A 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 eq. (5) is used to compute the magnetization of the spin configuration in our work. The last term in eq. (5) is used for theoretical calculation of magnetization.

$$M(N, T, \mu B) = < \sum_{i=1}^{N} s_i > = k_B T \frac{1}{\mu \mathrm{Z}} \frac{\partial}{\partial B} \mathrm{Z} \quad \ldots \quad (5)$$

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

Energy is the average Hamiltonian of the 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 the Ising system is governed by two terms. The first term with external field B is the self-energy term of spin when the spins experience field B. The later term which has coupler J incorporates interaction energy due to nearest neighboring spins.

$$E = < -\mu B \sum_i s_i - J \sum_{i,j} s_i s_j > = -\frac{\partial ln \mathrm{Z}}{\partial \beta} \quad \ldots (6)$$

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

$$C_v = \frac{\partial E}{\partial T} \quad \ldots (7)$$

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

$$C_v = \frac{<E^2> - <E>^2}{k_B T} \quad \ldots (8)$$

The behavior 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 found the value of critical point to be 2.269 $k_B T_c / J$. The magnetization at different ranges of temperature[5] is given by,

$$M(T) = \begin{cases} 0, & T > T_c \\ \{1 - [sinh^{-4} 2\beta\varepsilon]^{\frac{1}{8}}, & T < T_c \end{cases} \quad \ldots \quad (9)$$

Where, $\beta = 1/k_B T$ and interaction energy constant $\varepsilon = 1$.

Simulation Technique

Markov Chain Monte Carlo Algorithm

Monte Carlo method relies on use of random numbers and helps in probabilistic description of a problem. MCMC is a

sampling technique which leads us to desired phase space configuration corresponding 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 generating a random spin configuration with Boltzmann probability by making decisions to accept or reject random spin flips[11]. The loop shown in the flowchart of Figure 2 is implemented to generate a finite population of the representative configuration of spins in our lattice after certain nruns of thermalization, such that our samples attain stable values of magnetization for a particular temperature.

We will take a finite size of square or cubic lattice with 3x3 and 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 spins is randomly flipped and a 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 the history of Hamiltonian and Magnetization during nrun thermalizations which are 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 the simulation.

There are some limitations of the MCMC method. The computers generate pseudo-random numbers and the 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.

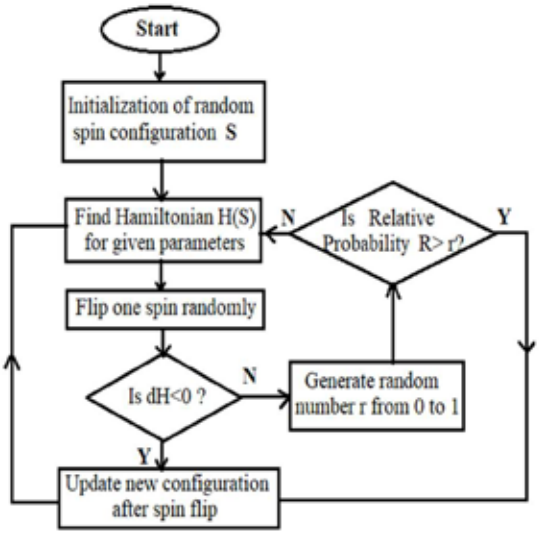

Figure 2: Flow-chart for MCMC thermalization.

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

1. Starting with arbitrary spin configuration
   $U_k = \{s_1, s_2, \ldots\ldots\ldots\ldots, s_N\}$
2. Generating a trial configuration U_{k+1} by picking a random spin s_i and flipping it $s_i \mapsto -s_i$
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 $H_{trial} > H_{Sk}$, 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.* $U_{k+1} = U_k$

Results and Discussion

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 figures 3 and figure 4 show that magnetization has been settled after a certain number of nruns.

Thermalization in 2D IM

Thermalization is the transition of arbitrary spin configuration towards a state with uniform energy for a particular temperature. We initialize the thermalization

algorithm with two types of configuration, first cold start (initialization with all spins +1) which is represented by black color, and hot start (with random spin configuration) , for which average magnetization begins with arbitrary values around zero as shown in the green color of figure 3. Only the thermalized samples will be considered for computation of thermodynamic quantities of interest.

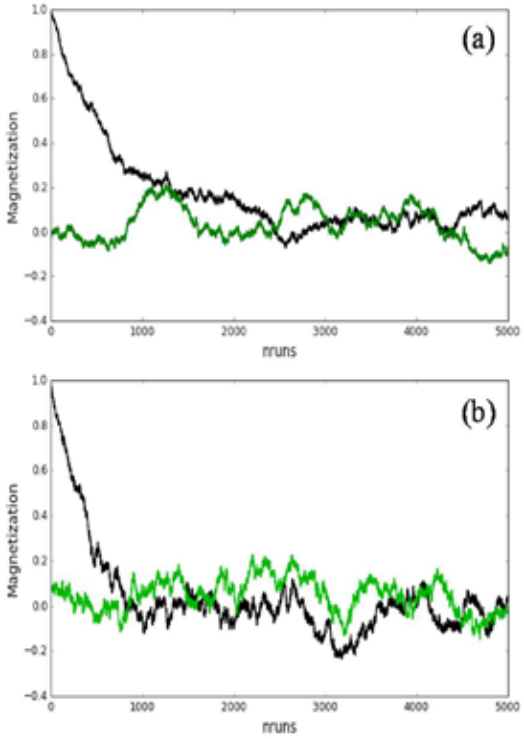

Figure 3: Thermalization in 2D IM (a) for lattice size L = 20 and (b) for lattice size L = 15 respectively. For both lattice size, thermalization was done at T = 6 J/k_B and field B = 0.

Figure 3(a) and 3(b) show 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. The evolution of the average magnetization in this case settles down to zero over 1500th nruns as shown in figure 3(a) and 3(b). Figures 4(a) and 4(b) show 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. We will plot the average of magnetization of such thermalized samples for discrete temperature points in the plot of magnetization as a function of temperature. We can observe the magnetization settles down after about 1500th runs of thermalization. To be sure that the sample we are taking represents a thermalized sample, we take samples 2000th nruns onwards for computation.

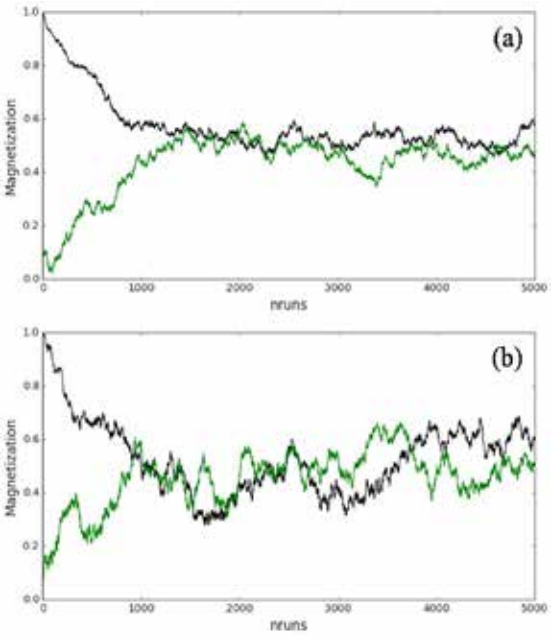

Figure 4: In 2D IM at B = 1, the thermalization at T = 5 J/K_B (a) for lattice size L = 20 and (b) for lattice size L = 15 respectively.

Findings of PhT in 2D IM

Bifurcation in magnetization below T_c shows symmetry breaking in the zero field at a 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 temperature has been observed where specific heat theoretically fails to be an analytic function of temperature[7] as shown in figure 5(b). In figure 5(a), the vertical red dotted line represents the critical temperature T_c = 2.269 J/k_B and the red scatter plot below T_c = 2.269 represents magnetization obtained through Huang's theoretical prediction. Critical temperature obtained from

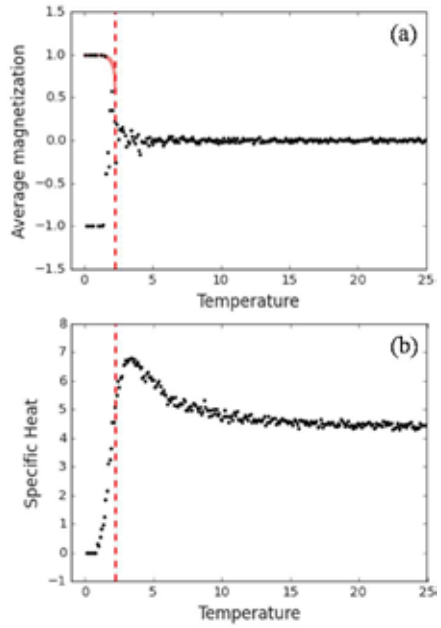

Figure 5: In 2D IM, at B = 0 (a) the temperature dependence of average magnetization and (b) the temperature dependence of specific heat.

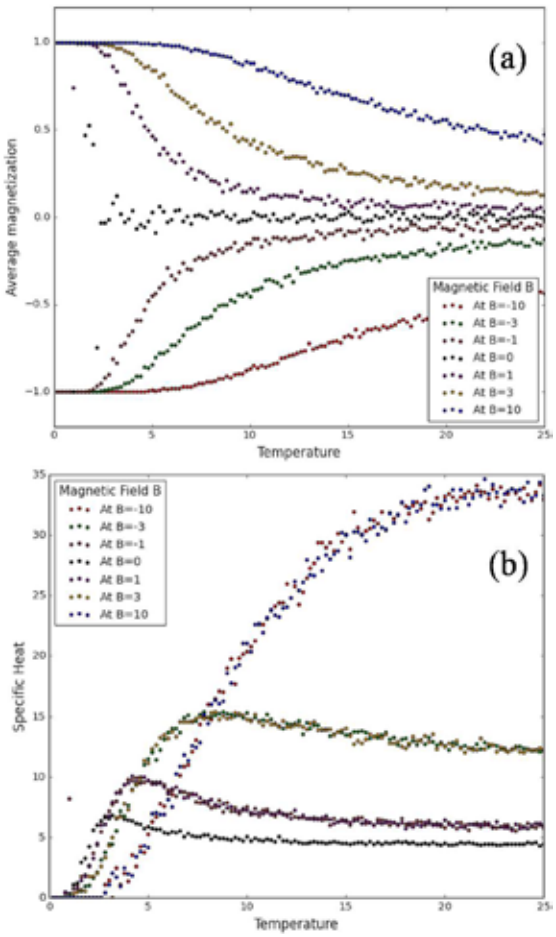

Figure 6: (a) The temperature dependence of average magnetization and (b) the temperature dependence of specific heat in 2D IM at different fields.

simulation is around $T_c = 2.2\ J/k_B$ consistent with Onsager's critical temperature of $T_c = 2.269\ J/k_B$. The hump of specific heat in figure 5 (b) has been observed behind the theoretical critical temperature represented by a vertical red dashed line.

Figures 6(a) and 6(b) show the average magnetization and specific heat at different external fields in 2D IM.

Simulation in 3D IM

27 spins were put in a 3x3x3 lattice with periodic boundary and thermalization was initiated. The figures 7(a) and 7(b) show that magnetization has been settled after 1500th nruns in thermalization of 3D Ising Model.

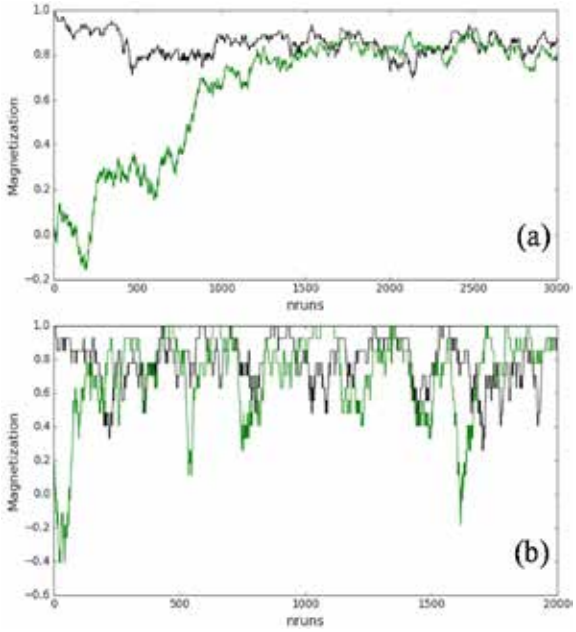

Figure 7: Thermalization at T = 5 J/K_B, B = 1 for lattice size (a) L = 5 and (b) L = 3 in 3D IM.

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.

Figures 7(a) and 7(b) show 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 a thermalized sample, we have taken samples 2000^{th} nrun onwards for computation.

Findings of PhT in 3D IM

In 3D IM, the simulation suggests critical temperature around T_c = 4.3 J/K_B which is shown in figure 8(a) and 8(b). It predicts specific heat increases on increasing temperature below T_c, falls down right after critical point and then attains nearly constant value on increasing temperature at B = 0 as observed in figure 8 (b).

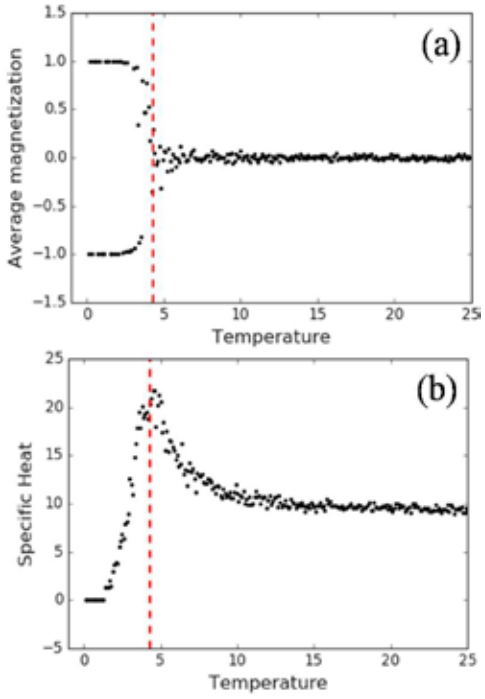

Figure 8: In 3D IM, at B = 0 (a) the temperature dependence of average magnetization and (b) the temperature dependence of specific heat.

A prominent hump has been observed in specific heat of 3D 'IM'. 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 an external field, with equal tendency to align in either +1 or -1 alignment. Average magnetization at a non-zero field shows a reflection symmetry along a line at B = 0 for curves of $\pm B$ like in 2D.

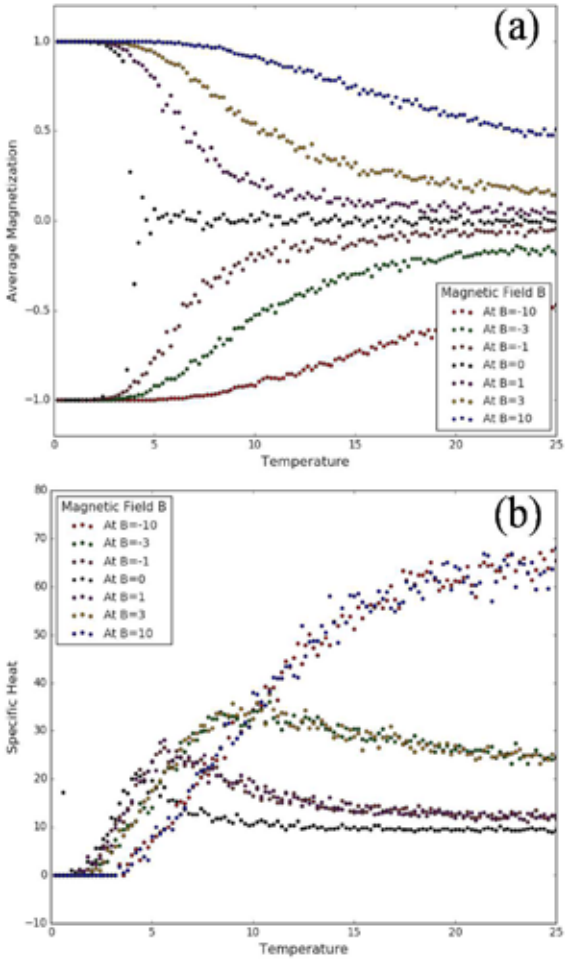

Figure 9: (a) The temperature dependence of average magnetization in 3D IM at different fields and (b) the temperature dependence of specific heat in 3D IM at different fields.

Figures 9(a) and 9(b) show the evolution of average magnetization at different fields on increasing temperature.

Comparison of PhT in 2D and 3D IM

The 3D model shows qualitatively the same results as the 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 the 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 a certain temperature, has been found to attain hump at the critical region. The scatter points of specific heat C_v are found to

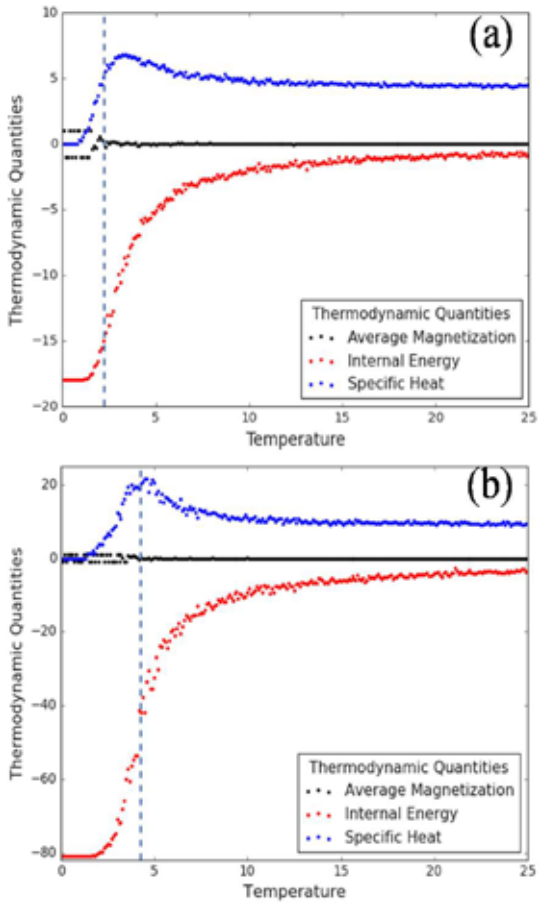

Figure 10: The temperature dependence of average magnetization (black), specific heat (blue) and energy (red) at zero field for 2D and 3D IM. (a) the vertical blue dashed line represents Onsager's critical point $T_c = 2.269\ k_B T_c/J$ in 2D and (b), the vertical blue dashed line represents critical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

overlap for external fields $\pm B$. Evolution of specific heat starts from zero at regime below T_c and grows to peak value at critical point. Specific heat lowers above critical point T_c and then attains a stable value as shown in blue scatter plot of figure 10(a) and 10(b). The fluctuation of energy of thermalized samples has increased on increasing magnitude of external field below critical temperature.

Conclusion

In simulation of phase transition of 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 all spins -1) in regions below critical temperature. Above critical temperature, either of the state collapse to a single state with random spin configuration in a system. In such a random spin configuration, the average magnetization takes values around zero due to the nearly equal number of +1 and -1 spins in the Ising system. This physically signifies the loss in magnetic property above critical temperature. Bifurcation of magnetization shows that the PhT in Ising model in 2D and higher dimensions exhibits the property of symmetry breaking. As the magnetization is significant in absence of an external field below T_c, this phenomenon has been attributed as spontaneous magnetization. At a non-zero field, the likelihood of spins to prefer certain alignment depends on the direction of the external field and magnitude of magnetization depends on magnitude of field $\pm B$. Temperature plays the role of increasing randomness of spins.

The plot of specific heat C_v as a function of temperature exhibits characteristic hump near critical regions. This shows that the fluctuation of energy in the Ising system is maximum in the region of phase transition. Our simulation observed in a small finite lattice of 2D has shown hump behind the theoretical critical point obtained by Onsager. On increasing the value of the external field, the hump of specific heat has shifted towards higher temperature. At extremely high temperature scales above criticality, it has been observed that the value of specific heat C_v attains constant values. In other words, as an effect of higher field, criticality has been delayed at evolving temperature regimes, followed by delayed stability of C_v over evolving temperature scales. The pattern of rise and fall observed in C_v has been found to be dependent on the region of evolving temperature scale, separated by critical point T_c. This phenomenon is prominent both in 2D and 3D.

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