

The Ising Model for Calculation Energy and Magnetization in Magnetic Fields (B=0, B≠0) for different Lattice Sizes

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Abstract

Two dimensional Ising model's partial transition location has been determined with significant samples using Monte Carlo method. The magnetization per site (μ) and the energy per site (j),heat capacity (CV), susceptibility (x)of a ferromagnetic substance are calculated as a function of inverse temperature (βJ) for different lattice sizes, in magnetic fields (B=0,B≠0). The critical inverse temperature (βC=0.435 KB/J) has been determined. The precise partition functions (i.e. precise solutions) of the Ising model in $(L \times L = 4, 8, 16, 32)$ the square lattice sizes with free boarders stipulations are acquired after categorize all 2L×L=216×16 (≈1.157×1077) and 232×32 (≈1.79×10308) shapes of spin and we observe how the system evolves across steps to achieve balance. Moreover, the stage of transitions and critical conditions have been discussed using the precise partition function in $(L \times L=16, 32)$ square lattice sizes with free boarders stipulations.

Key Words: Ferromagnetic Material, Ising Model, Monte Carlo Steps, Metropolis Algorithm Method. **DOI Number: 10.14704/nq.2020.18.2.NQ20120 NeuroQuantology 2020; 18(2):23-31**

Introduction

Basically the partial a stage transitions and critical conditions are the foremost wide phenomenon in nature. The square-lattice sizes (*L*2) of the Ising model are the simplest efficient system appears partial transitions (the partial a stage transitions between the paramagnetic and ferromagnetic phase) and critical condition at limited temperatures. The square-lattice sizes (*L*2) Ising model has played a central role in the understanding of stage transitions and critical conditions [1,2]. The precise solution for square lattice sizes of the ising model with periodic stipulations is well known both in the thermodynamic limit (that is, the unlimited size system) [3] and limited system. However, the precise solution of the square-lattice sizes (*L*2) Ising model with free boarders stipulations is not known

for an arbitrary size system.

Previous study has been well done on two dimensional Ising model of ferromagnetic. Bhanot [4] evaluated the precise partition functions of the Ising model in (*L*2) square lattice sizes with free boarders stipulations up to (*L*=10) using Cray XMP. Bhanot counted all $2^{L \times L} = 2^{100}$ (≈ 1.27 x 10³⁰) states for (*L*=10), and start-up get to some beneficial outcomes. Stodolsky and Wosiek [5] obtained the precise partition function for $L = 13$ (corresponding to 2^{169} ≈ 7.48 x 10⁵⁰ states) using IBM RISC 6000, and studied stage transitions based on the entropy as a function of the energy. Seung-Yeon Kim [1] computed the precise partition function of the Ising model on square lattice sizes with free boarders stipulationsfor (corresponding to states) using the micro canonical convey matrix.

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In this study, the precise partition function and emulate the critical conditions of ferromagnetic substances in (*L×L*) square lattices with free boarders stipulations for (*L*×*L*=16) and (*L×L*=32) have been calculated. The average energy, average magnetization and the average absolute magnetization have been calculated as a function of inverse temperature (*βJ*) and determining the critical inverse temperature $(\beta_C=0.435 K_B/\gamma)$ in a magnetic field (*B*=0, *B*≠0) fora (*L×L*= 4, 8, 16, 32) square lattice sizes.

The Ising Model

Hamiltonian system depends on the order of the grid spins and we conclude from this characteristics, for example, magnetization [6,7]. Let *Si,j* denote a spin in lattice coordinates *i* and *j* with either spin up or spin down, $S_{i,j}= \pm 1$. Assume which Hamiltonian is:

$$
H = -J \sum_{\langle ij \rangle} s_i \ s_j - B \sum_i \ s_{i \ (1)}
$$

where<*ij*>an strategy that sums up over the closest neighboring spin pair because the spin at location*ij* interacts with spins at locations *i*(*j±*1) and *j*(*i±*1) respectively. J_{ii} is the exchange energy between the spins and *B* is an external magnetic field. In the absence of an external magnetic field, *B = 0*, and so the Hamiltonian reduces to[8]

$$
H = -J \sum_{\langle ij \rangle} s_i \, s_j \tag{2}
$$

The following distribution of probabilities should be used to calculate the expected values such as mean energy $|E\rangle$ or magnetization M \rangle in thermodynamic physics at a specific temperature

$$
P_i(\beta) = \frac{e^{-\beta E_i}}{Z} (3)
$$

with $\beta = 1/K_B T$ is the inverse temperature, K_B the Boltzmann constant, *Eⁱ* the energy of state *i*, whereas *Z* the partition function for the canonical ensemble we may write

$$
Z=\sum_{i=1}^M e^{-\beta E_i},
$$

The specified configuration energy is given *i* by

$$
E_i = -J \sum_{\langle i j \rangle}^{N} s_j s_i
$$

Computational Observables

For getting the result, I have altered the Fortran 90 And

code that was developed by Lisa Larimore [9]. We can measure of the effect inverse temperature (*βJ*) on the energy and the magnetization, heat capacity (C_V) , susceptibility (x) at each step, the critical inverse temperature $(\beta_C=0.435K_B/J)$ has been determined. Then, by taking the amount of all the spins in the lattice, we can evaluate the magnetization as a function of the Monte Carlo simulation (*MCS*). Two dimensional shapes are plotted using Grapher version 1.09 [10]. The computational observables of special concern are $\langle E \rangle^2$, $\langle |M| \rangle^2$ and $\langle M \rangle^2$. We determine in the next method:

$$
\langle M \rangle = \frac{1}{N} \sum_{s}^{N} M(s) \tag{4}
$$

Where $\langle M \rangle$: represented the mean magnetization and $M(s)$, the magnetization per spin.

To calculate the energy provided in equation (1), we use the Hamiltonian

$$
\langle E \rangle = \frac{1}{2} \langle \sum_{i}^{N} H_{i} \rangle = \frac{1}{2} \langle -J \sum_{i}^{N} \sum_{jnn} S_{i} S_{j} \rangle
$$
 (5)

fact that every pair is calculated twice in the sum. 24 the factor of $(1/2)$ is presented accounting for the Equation (4) is utilized in an analogous method to find $\langle E^2 \rangle$. We anticipate a noticeable flip-flop in these amounts at the critical temperature.

The equilibrium of the scheme can be depicted by the following quantities: [11-13]

• Heat Capacity
$$
(C_v)
$$
:
\n
$$
C_V = \frac{1}{N^2} (1/kT)^2 ((E^2) - \langle E \rangle^2)
$$

It is linked to the variance of the energy.

• Susceptibility (χ)

 $k_B T$

$$
\chi = \frac{1}{N^2} \frac{J}{kT} \left(\langle S^2 \rangle - \langle S \rangle^2 \right) \tag{7}
$$

Where $S = \sum_j S_j$. It is related to the difference of the magnetization.

The free energy can come from the equation [13, 14]**:**

$$
F = -k_B T \ln Z = \langle E \rangle - TS \qquad (8)
$$

\n
$$
Z = \sum_{S_j} e^{-\beta E(S_i)}
$$

\n
$$
\beta = \frac{1}{1 - \beta}
$$

(6)

The system approaches to the equilibrium by minimizing F (the free energy).

Fluctuations in Monte Carlo Time "Evolution"

In the simulation system, whenever the flip is done, the interaction energy will be reduced. If the energy increases, the flip is only obliged with an eventuality of $\{exp(-\beta E)\}$ whereby $(\beta=1/K_B T)$ and (*E>0*) is the energy variance between upturned and non-upturned case (metropolis algorithm method).The applicable temperature will be in modules of (*βJ*) named the decreased temperature and is the "natural" temperature module used for the While of the execution. The emulation time repeatedly calculates what is called (Monte-Carlo Step), generally indicated to as time, each of which involves the potential flipping of all spins within the vicinity [15].

Simple Sampling

The essential elementary sampling manner comprises of simply randomly selecting points within the configuration space from anywhere. A huge numeral of spins patterns is generated randomly (for the whole lattice) and data are used to calculate the average energy and magnetization. However, this mechanism needs to suffer from precisely the same problems as the quadrature manner, often sampling from unimportant areas of the stage size.The chances of producing a randomly created spin array and up / down spin patterns are remote (-2^{-L}) , and high-temperature random spin array is highly likely. The most common way to avoiding this problem is by using the Metropolis importance sampling, which works by applying weights to the microstates [16].

Boundary conditions for inverse temperature (βJ)

For a given β = $(K_B T)^{-1}$, the initiation lattice is set as the settled lattice of the former (*β*):

- At $(\beta = (K_B T)^{-1} = 1)$, i.e. at a fully low temperature, completely aligned spins are obtained. There is maximum magnetization. Then, as the temperature will increase the change of spins gradually.
- When $(\beta = (K_B T)^{-1})$ is such that $\beta \approx \beta_c$ there are various clusters of aligned spins, magnetization is utmost in each cluster, however, the magnetization of the group is generally cancelled due to the eventuality of being in the α_i configuration is equal to the eventuality of being in the **-αi**configuration.

 The dipoles are routed randomly at a fairly high temperature (β = (K_B *T*)⁻¹=0), while the lattice is initialized at every value of (*β*= $(K_B T)^{-1}$), the findings differ: At a totally low temperature, there are several clusters of aligned spins. These domains stop evolution: We usually tend to get domain names from Weiss and walls Bloch. As a consequence, magnetization is random. The matrix of size limits the number of possible clusters [13].

Results and Discussion

Location of the critical transition phenomenon

Critical region shows the maximum temperature of non-zero magnetization. In this situation, the system is subject to transition called partial transition (a stage transition) from order-todisorder [17]. In order to locate the essential (critical) inverse temperature (*βC*), the most realistic value is given in the thermodynamic limit, where $(L \times L = N^2)$, the boundary of infinity is regarded. Thus, we aimed to calculate the essential (critical) inverse temperature with fully different lattice sizes. Figure (1) shows the critical inverse temperature as *N* approaches infinity, andhas been calculated the critical region for many lattice sizes and it value $(\beta_C=0.435K_B/I)$ without effect of the magnetic field (*B=0*).

Figure 1. Critical inverse temperature ($β$ ^{*C*}=0.435)</sup> depend on different lattice sizes

Fluctuations in Monte Carlo technique

Collected communiques for lattice size (L=4) can be clarified in figure 2. Thesecommuniques are done at a temperature minimal than the critical inverse temperature $\beta_c J$. We can expect a settled state to existand nonetheless it is plainly displaying a flip-flopwhich is uncommon, resulting in an entire

flip of the magnetization. The flip-flop (fluctuation) happens prior (5000 *MCS*) and the magnetization summits at (0 from −1). The arrangement is here in the center of the ravine and occurs to return to its prior state. The similar state happens simply after (5000 *MCS*) however in this case selects to flip to an reverse, but evenly likely, magnetization, from (- 1 to 1).

Figure 2. This planned indicates a spontaneous permutation (flip) in magnetization for a (L=4) lattice size at $\left(T^{-1}=1\right)$

Magnetic field status (*B=0***)**

Impact of the magnitude at the distinguishing

amounts

To sight the impacts of the magnitude (size) of the lattice on the transition of the stage, the thermodynamic amounts are plotted in (*L×L*=4, 8, 16, 32) without effect of the magnetic field (*B=0*). We began with random spin at the lattice places and used Ising model to calculate magnetization and energy as noted in tables 1,2 Appendix (A). We executed Metropolis algorithm Monte Carlo simulation of an Ising Model in Fortran 90 Code. The emulations were in (*L×L*= 4, 8, 16, 32) the square lattice sizes with free boarders stipulations, and the simulation for inverse temperature (*β*) of a 0.09 K_B /*J* through 1.4 K_B /*J* with intervals of 0.02. As the temperature raise, the system was allowed to equilibrate for 10,000 steps, and then the averages were performed over the entire lattice. The effect of inverse temperature (*β*) in (*L*×*L*= 4, 8, 16, 32) different lattice sizes on average absolute magnetization $\langle \vert M \vert \rangle^2$, average magnetization $\langle M \rangle^2$ and susceptibility (*x*) have been shown in figure (3a, 3b, 3c, 3d).

Figure 3. Variations in the normalized worths of with $\langle M \rangle^2$, $\big\langle |M|\big\rangle^2$ and susceptibility χ as a function of the inverse temperature at (a) L=4, (b) L=8, (c) L=16, (d) L=32 in an external field $(B = 0)$.

Our automatic permutation findings, as shown in figure (2), show that this would lead to an averaging out of the mean magnetization $\langle M \rangle$. This naturally hasa harmful influence on account the disparity of the magnetization and thus the susceptibility. This can be illustrated in the figure (3), the drawing appears that $\langle M \rangle^2$ remain steady or zero at low temperatures (high inverse temperature βJ) for approximately a prolonged duration. This would explain the disparity at *βJ* greater inverse temperature to summit (peak). Despite the big size of the latticethe automatic magnetizationis fewer probable to happen and the critical point moves gradually to low inverse temperature *βJ* which means that the summit for the susceptibility will be approaching the Curie temperature (critical inverse temperature β_c =0.435 K_B /*I*) from the left. We deduce that the bigger the numeral of *MCS* we use the more probable we are to insert automatic permutation and then averaging out of the mean magnetization that couldchange the location of the summit (peak) of the susceptibility further to the left. Workaround for this issue, that is, there is egalitarian eventuality for the magnetization to change to an adverse arrangement or revert to its prior arrangement.

To calculate the average absolute magnetization $\left\langle M\right\vert \right\rangle ^{2}$ only one likelihood summit (positive one) will be actively considered and the multipliers will be overcome by averaging out the mean magnetization. This is evident from the reality that formerly we have recurrent flip-flops, in figure (2),

between peak positive and negative magnetization at low inverse temperatures resulting in a zero mean magnetization. However positive worths to regard for the averaging of the mean magnetization producing a non zero average. This influene is fewered somewhat because the ravine is raised at low inverse temperatures resulting in the magnetization having a rise likelihood of being close to zero. Happily, this nonzero average for the magnetization at higher temperatures is illogical since it doesnot impact the Curie temperature and shows solely in the zone which is above it. Figure (4a, 4b), the average energy $\langle E \rangle^2$ and heat capacity (C_V) against the inverse temperature in $(L \times L = 4, 8, 1)$ 16, 32) lattice sizes are shown. As the lattice size smaller, the more complicated to see an abrupt increasing as in (*L×L*=4, 8) lattice sizes, the sharp gradient of smaller lattices indicates at a probable but not obviously explained phase change.The curve of the diagram gets clearer with the increase in lattice size thus, (*L×L*=16, 32) lattice sizes their results were nearly identical. The average energy is minimal and it increases slowly as the temperature rises. At a given temperature, the energy increases significantly finally approaches 0*J*. The heat capacity (C_V) has a summit that symbolizes the phase change. At low inverse temperature *βJ* (high temperatures), it decreases until it reaches 0. While ata high inverse temperature *βJ* (low temperatures), the more of the peaks marking the phase change clearly.

Figure 4. Average energy & heat capacity versus the inverse temperature in two lattice sizes (a) L=16,(b) L=32 at an external field $(B=0)$.

Magnetic Field Status *(B≠0)*

Thermodynamic amounts against the magnetic field (B≠0)

The effects of the presence of the magnetic field (*B≠0*) on the thermodynamic quantities have been also investigated. The effect of the magnetic field on the average absolute magnetization $\langle\vert M\vert\rangle^2$, average magnetization $\left\langle M\right\rangle^2$, and average energy $\left\langle E\right\rangle^2$ as a function of inverse temperature (*βJ*) for (*L×L*=16, 32) lattice sizes have been shown in figures (5 and

Figure 5. The impact of the external magnetic field $(B \neq 0)$ in the average energy & heat capacity in two lattice sizes, (a) L=16, (b) L=32.

Figure (5a, 5b) shows the average energy $\langle E\rangle^2$ per spin as a function for inverse temperature*βJ*. At (*β*<*βC*) the energy per spin is relatively high as expectedforindiscriminate arrangementdue to thermic agitation which prevents alignment spins with the influencer external magnetic field (*B≠0*), where a sit at (*β*>*βC*) settle to a

$$
{(\langle E \rangle)^2 / N = 0.035 J = -0.035, \quad {\langle E \rangle}^2 / N = -0.0083 J = -
$$

0.0083}. This indicates that all spins are line up in the parallel. But regarding to the heat capacity (C_V) getswith clearer for different lattice sizes, the peaks a decrease for the heat capacity can be observed in (*L×L*=16) and (*L×L*=32) lattice sizes which leads toa little dislodging in the locations of the peaksatthe

low values for the inverse temperature *βJ*. Figure (6) shows the average magnetization $\langle M \rangle^2$ and the average absolute magnetization $\left\langle \left| M \right| \right\rangle^2$ as a function for inverse temperature *βJ*. At (*β*>*βC*), the average magnetization $\langle M \rangle^2$ average absolute magnetization $\langle M|\rangle^2$ are high values and is consistent with the results because the sequence particles is long in lattice and the system takes

greater time reach equilibrium, which means it evolves over bigger numeral of steps, while at (*β*<*βC*) they are less due to thermic agitation which preventsalignment spins with the effecter external magnetic field (*B≠0*). As for the susceptibility χ against the inverse temperature (*βJ*), the magnetic field causes a decreasing in the magnitude of the peaksdue to thermic agitation which neglectsthe effect of the presence of the magnetic field (*B≠0*).

Figure 6. The impact of the external magnetic field $(B\neq 0)$ in the magnetization and susceptibility in two lattice sizes

Conclusion

The Monte Carlo method implemented in the Ising Model that prescribes the magnetic characteristics of the substances permit obtaining the thermodynamic quantities variation. The squarelattice size (*L2*) Ising Model is the simplest system showing partial transitions (the transition between the ferromagnetic phase and the paramagnetic section) and critical conditions at limited temperatures. Under a certain temperature (critical inverse temperature *βc=*0.435 *KB/J*), the material will be in the paramagnetic state, which means that the average magnetization decreases and the average energy increases, while above a certain temperature (critical inverse temperature *βc*=0.435*KB/J*) the material will be in the case of ferromagnetic, thus, the average magnetization increases and the average energy decreases. Moreover, under a certain temperature (critical inverse temperature *βc*=0.435 *KB/J*), spontaneous magnetization is zero. The precise partition functions (that is to say, the precise solutions) of the Ising model in (*L×L*=4, 8, 16, 32) of a ferromagnetic square lattice, is unknown with free

boarders stipulations for arbitrarily sized systems. The precise partition functions of the Ising model on the (*L×L*=16), (*L×L*=32) lattice sizesin 2D Ising model for simulation of critical situation using Monte Carlo method have been obtained. We have too debated the stage transitions and critical conditions of the square lattice IsingModel using the precise solution on the square lattice with free boarders stipulations, it is as follows:

- At the absence of the external magnetic field (*B*=0), a stage transition at the critical inverse temperature (β_c) is powerfully marked. This transition separates (*β*>*βC*), wherever the magnetization (*M*) is maximum, the spins are aligned, and $(\beta < \beta_C)$ wherever the magnetization (*M*=0), the spins are at random oriented.
- At the presence of the magnetic field $(B \neq 0)$, phase change (phase transition) isn't thus marked. At (*β*<*βC*) a very low inverse temperature (high temperature), the field has no impact as a result of the thermic incitement. In a very public method, the spins are aligned with the external magnetic field, however at (*β*>*βC*) thealters of trend

occurs solely if the field is below the critical point.

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Appendix (A)

Table 1. Calculation magnetization as a function of inverse temperature (Beta) at (*L*×*L*=16×16) lattice size in external magnetic fielf (*B=0*)

30

Table 2. Calculation energy as a function of inverse temperature (Beta) at (*L*×*L*=16×16) lattice size in external magnetic fielf (*B=0*)

