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Two Dimensional Ising Model Application With MONTE CARLO Method

Dhia`a K. Khudier * **Nabeil A. Fawaz****

*Universityof Al –anbar, College of pharmacy
**University of Al – anbar, College of science

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ABSTRACT

The location of the phase transition in the two dimensional Ising model were determined using Monte Carlo simulation with importance sampling. The *magnetization* (M) *per site* (μ), *energy* (E) *per site* (J), *magnetic susceptibility* (χ), *specific heat* (C_V) of a Ferromagnetic materials were calculated as a function of temperature T for $(16 \times 16\,, 30 \times 30\,, 55 \times 55)$ spin lattice interaction in zero and nonzero magnetic field $(B = 0, B \neq 0)$. There is thus a phase transition defined by the Curie temperature. The Monte Carlo method was used to check the results and to confirm the phase transition . The internal interaction results were found to be consistent with what was expected. As a magnetic field is applied, the spins tend to align with it for $T > T_C$ and its effect is not significant at a very high temperature because of the thermal agitation. For $T < T_C$, the alignment of the spins is possible only if the amplitude of the field is big enough.

Introduction

The ising model allows to deal with thermodynamic problems such as the behavior of the spins in ferromagnetic materials. Thus, referring to a two-dimensional lattice of 1/2 spins to which the Monte Carlo method is applied, we determine the observables describing the system and their evolution with the variation of the magnetic field and the temperature [1].

An ising model is introduced and used to investigate the properties of a Ferro magnet with respect to its magnetization and energy at varying temperatures.

* Corresponding author at: University of Al–anbar, College of pharmacy. E-mail address:

The observables are calculated and a phase transition at a critical temperature is also illustrated and evaluated [2]. we can to rely on numerical methods that adopted is based on program as (Fortran code 90),to build the phase diagrams .

In most ordinary materials the associated magnetic dipoles of the atoms have a random orientation. In effect this non-specific distribution results in no overall macroscopic magnetic moment.

However in certain cases, such as iron, a magnetic moment is produced as a result of a preferred alignment of the atomic spins [2].

This phenomenon is based on two fundamental principles, namely energy minimization and entropy maximization. These are competing principles and are important in moderating the overall effect.

Temperature is the mediator between these opposing elements and ultimately determines which will be more dominant. The relative importance of the energy minimization and entropy maximization is governed in nature by a specific probability[2,3].

$$P(\alpha) = \exp \frac{-E(\alpha)}{kT} \qquad (1)$$

Where $E(\alpha)$: the energy ,

$P(\alpha)$: Partition function ,

T : Temperature ,

k : Boltzmann constant

which is illustrated in figure 1 and is known as the Gibbs distribution

Theory And Method

The ising model

The Hamiltonian for a system that is dependent on the arrangement of spins on a lattice and from that we can deduce properties such as magnetization and susceptibility [4,5]. Suppose that the Hamiltonian is

$$H = -J \sum_{\langle i\, j \rangle} s_i\, s_j - B \sum_i s_i \qquad (2)$$

internal interaction energy external magnetic energy

where $\langle i\, j \rangle$ means that we sum over the nearest-neighbor pair of spins. This means that the spin at site $i\, j$ interacts with spins at sites $i(j \pm 1)$ and $j(i \pm 1)$ respectively. We are assuming periodic boundary conditions in our model which means that every spin will interact with four other spins regardless of their position on the finite lattice. The better understanding of the proposed system can be seen as in figure 2 .

Here J is the dimensionless interaction strength and B represents the energy involved in the magnetization of the lattice and is also dimensionless.

The Ising Model considers the problem in two dimensions and places dipole spins at regular lattice points while restricting their spin axis to be either up (+y) or down (-y). The lattice configuration is square with dimensions L and the total number of spins equal to $N = L \times L$. In its simplest form the interaction range amongst the dipoles is restricted to immediately adjacent sites (nearest neighbors). This produces a Hamiltonian for a specific spin site, i , of the form [2,6] :

$$H_i = -J \sum_{jnn} s_i\, s_j \qquad (3)$$

where the sum j_{nn} runs over the nearest neighbors of i . The coupling constant between nearest neighbors is represented by J while the S_i and S_j are the respective nearest neighbor spins. The nature of the interaction in the model is all contained in the sign of the interaction coupling constant J .

If J is positive it would mean that the material has a ferromagnetic nature (parallel alignment) while a negative sign would imply that the material is antiferromagnetic (favors anti-parallel alignment). J will be taken to be $+1$ in our discussion and the values for spins will be $+1$ for spin up and -1 for spin down. A further simplification is made in that J/k_B is taken to be unity. The relative positioning of nearest neighbors of spins is shown in figure 3 with the darker dot being interacted on by its surrounding neighbors [2].

The equilibrium of the system can be represented with these quantities [1,5,6].

- ***Magnetization***

$$M = \frac{1}{N^2} S \qquad (4)$$

N^2**: The total no. square of spins** S **.**

- ***Heat capacity***

$$C = \frac{1}{N^2}(1/kT)^2\left(\langle E^2\rangle - \langle E\rangle^2\right) \qquad (5)$$

$\langle E\rangle^2$**: Average of the energy square of spins .**

T**: Temperature ,** k**: Boltzmann constant**

It is linked to the variance of the energy.

- ***Susceptibility***

$$\chi = \frac{1}{N^2}\frac{J}{kT}\left(\langle S^2\rangle - \langle S\rangle^2\right) \qquad (6)$$

T**: Temperature ,** k**: Boltzmann constant**

J**: is the dimensionless interaction strength .**

where $S = \sum_j S_j$. It is linked to the variance of the magnetization .

The free energy should satisfies the equation**:[1,5]**

$$F = -k_B T \ln Z = \langle E\rangle - T S \qquad (7)$$

Where $Z = \sum_{\alpha_j} e^{-\beta E(\alpha_j)}$

Z**: partition function**

and $\beta = \frac{1}{k_B T}$

Where $\beta =$ **the Boltzmann factor is equal to unity .**

The system approaches the equilib- rium by minimizing F.

- At low temperatures, the interaction between the spins seems to be strong, the spins tend to align with another. In this case, the magnetization reaches its maximal value $|M| = 1$ according to its formula, the magnetization exists even if there is no external magnetic field.
- At high temperature, the interaction is weak, the spins are randomly up or down. So, the magnetization is close to the value $M = 0$. Several configurations suits: the system is metastable.
- The magnetization disappears at a given temperature.
- Thus there exists thus a transition phase. In zero external magnetic field, the critical temperature is the Curie temperature $T_C = \frac{2}{\ln\left(1+\sqrt{2}\right)}$ (obtained by the Onsager's theory) [1,7]. According to the transition phase theory, the second order derivative of the free energy in B and in T are discontinuous at the transition phase; as the susceptibility and the heat capacity are expressed with these derivatives, they should diverge at the critical temperature.

Behavior of the spins

For a given (β), the starting lattice is defined as the stable lattice of the previous (β) :

- At $(\beta = 1)$, i.e. at a very low temperature, we obtain fully aligned spins.
  The magnetization is maximum. Then, as the temperature increases the spins are gradually changed.
- When (β) is such that $T \approx T_C$, there are several clusters of aligned spins, in each cluster the magnetization is maximum but the magnetization of the set is null in general because the probability which will be in the configuration α_i is equal to the probability that will be in the configuration $-\alpha_i$.
- At very high temperature $(\beta = 0)$, the dipoles are randomly oriented.

When the lattice is initialized at each value of (β), the results are different: At a very low temperature, there are several clusters of aligned spins. These domains stop to evolve: We obtain Weiss domains and Bloch walls. The magnetization is thus

random. The size of the matrix limits the possible number of clusters.[1]

Results And Discussion

Case of zero external magnetic field

Influence of the size on the characteristic quantities :

In order to see the effects of the size of the lattice on the transition of the phase, the thermodynamic quantities are plotted for several sizes in the absence of magnetic field. We notice that if the size is not big enough, the phase transition is not really perceptible. The effect of temperature for different lattice sizes on energy and magnetization have been shown in figures (4 and 5) .

At very low temperatures, the energy is minimum and it slowly increases with the temperature. At a given temperature, the slope for three different sizes of lattice becomes the same abrupt increasing and the energy finally approaches $(0\,J)$.

For the three sizes, the magnetization is maximum at low temperatures and at Curie temperature $T_C = 2.65 \pm 0.05$ for

lattices $(16\times16\,,30\times30)$, but at $T_C = 2 \pm 0.2$ for lattice (55×55) the magnetization becomes minimum because the sequence particles is long in lattice as well as it takes greater time for a larger system to reach equilibrium which means that must be let the system evolve over a larger number of steps. There is a transition such that the magnetization above this temperature is almost null.

The bigger is the lattice , the faster is the demagnetization . Moreover, the demagnetization is not complete at small sizes, in this case $(M)$is constant and non-null at high temperature. Indeed, there are finite size effects[1]. Therefore, a lattice (30×30) is appropriated to determine the transition phase according to the above discussion.

The heat capacity and the susceptibility against the temperature for different sizes have been shown in figures (6 and 7), respectively .

The heat capacity has a peak at Curie temperature $T_C = 2.45 \pm 0.2$ which symbolizes the phase transition, at high temperatures, it decreases until it reaches 0. The bigger the lattice is, the more the peaks marking the phase transition are pronounced.

The peak is present in the figure (7) as well at $T_C = 2.5 \pm 0.10$, but the susceptibility becomes almost null at high temperatures.

The finite size effects for a lattice (30×30) is appropriated to determine the transition phase. When the size is appropriated enough, the susceptibility and the heat capacity diverge, and this is consistent with the theory.

Influence of the magnetic field

Thermodynamic quantities against the temperature :

The effect of the external magnetic field $(B \neq 0)$ on the thermodynamic quantities have been also investigated . In figure (8) the influence of the magnetic field on the energy makes the shift of the energy less abrupt with a lattice (30×30).

In figure (9) the magnetization is in general bigger when a magnetic field is applied, but at high temperatures, the magnetic field has only little effect.

The heat capacity and the susceptibility against the temperature for a lattice (30×30) and with presence of the external magnetic field $(B \neq 0)$ have been shown in figures (10 and 11), respectively .

The temperature at the location of the peak, is lightly displaced toward the bigger values.

In figure (11) the magnetic field generates a decreasing in the magnitude of the peak. At high temperature, the magnetic field has almost no effect. The thermal agitation makes negligible effect in the magnetic field.

The bigger the lattice is, the more the peaks marking the phase transition are pronounced.

Thermodynamics quantities against the magnetic field

The effect of the external magnetic field $(B \neq 0)$ on the thermodynamic quantities with a lattice (30×30) have been shown in figures (12 and 13), respectively. The influence of the magnetic field on the energy and magnetization at several given temperatures, the magnetic field varies from $(\mu B = +1J)$, a large positive value to $(\mu B = -1J)$, a large negative value .

Both the energy and magnetization quantities are approximately null constants as shown in figures (12 and 13), respectively. The magnetic field cannot establish an order, the temperature is much too high, it confirms the above results about the influence of the magnetic field according to the temperature.

The effect of external magnetic field $(B \neq 0)$ on energy and on the magnetization with a lattice (30×30)have been shown in figures (14 and 15), respectively .

As shown in figure (14), the magnetic field has a large positive value at the beginning ,whereas the energy is negative , the spins are thus up, they align with the magnetic field. Then the energy increases linearly with (μB) until the sign of the magnetic field changes. the magnetic field becomes a large negative value, but the energy is negative and maximum, the spins are down, they align with the magnetic field. Then the energy decreases linearly with (μB). The energy quantity follow the pattern from $(\mu B = -1J)$ to $(\mu B = 1J)$.

In figure (15) at the beginning , the magnetic field has a large positive value, the magnetization is positive and maximum, the spins are up, they align with the magnetic field. Then the magnetization decreases with (μB) until the sign of the magnetic field changes. The magnetization becomes negative. the spins tend to align with the magnetic field and the magnetization increase with (μB). The magnetization quantity follow the same pattern from $(\mu B = -1J)$ to $(\mu B = 1J)$ as shown in figure (14).

Conclusions

The Monte Carlo method applied to the Ising model which describes the magnetic properties of materials allows to obtain the thermodynamic quantities variations. The results are consistent with the expected values and behavior in the case where the lattice is big enough to limit the finite size effect [1]. At a certain temperature ($T>T_C$) and in the absence of magnetic field (B), the spins are randomly oriented, a phase transition will be in ferromagnetic state, Therefore the average magnetization will be decreased and the energy state increases, while below a certain temperature at ($T < T_C$) the spins are aligned, hence a phase transition will be in a ferromagnetic state, and the average magnetization will be increased and the energy state decreases. Moreover, above a certain temperature spontaneous magnetization (M) will be zero.

In the presence of a magnetic field (B), the phase transition is not so marked. At a very high temperature, the field has no effect because of the thermal agitation. In a general way, the spins align with the magnetic field but at ($T < T_C$) the changes of

direction happens only if the field is above a critical value .

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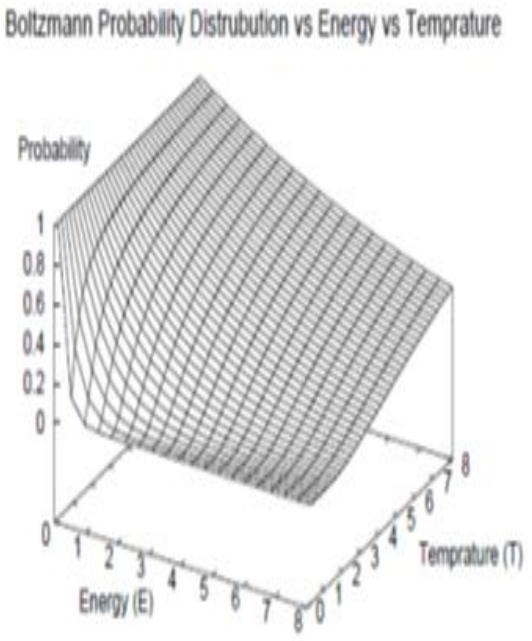

Figure 1: shows the Boltzmann probability distribution as a landscape for varying Energy (E) and Temperature (T) [2] .

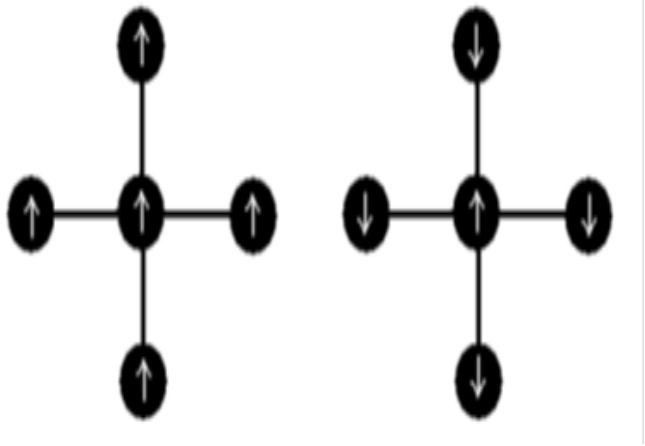

Figure 2: The energy of particle on the left is low since all the neighboring particles have the same alignment of spin. In contrast, the energy of the particle on the right is at its highest since all the neighboring particles have a different spin alignment [4].

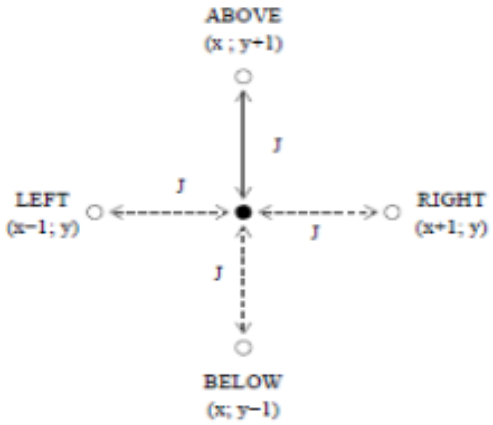

Figure 3: Nearest neighbor coupling. The dark dot, at position(x,y), is being interacted upon by its nearest neighbors which are one lattice spacing away from it [2].

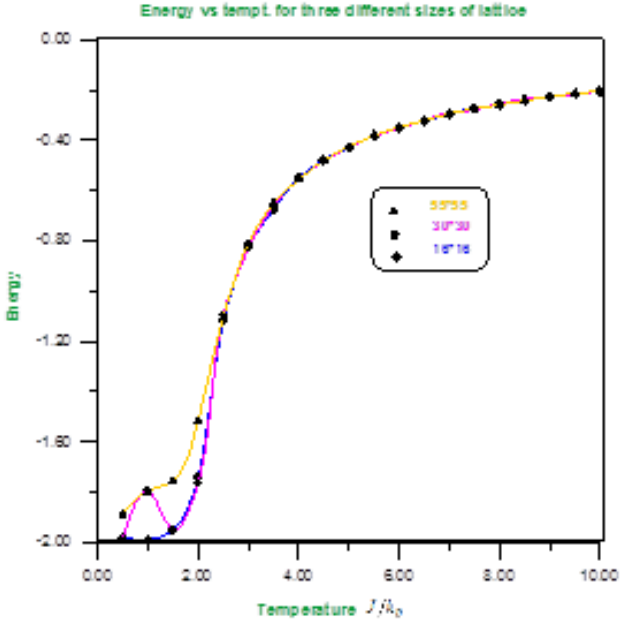

Figure 4: Energy (in J-unity) against the temperature for three different sizes of lattice for case of zero external field (B=0).

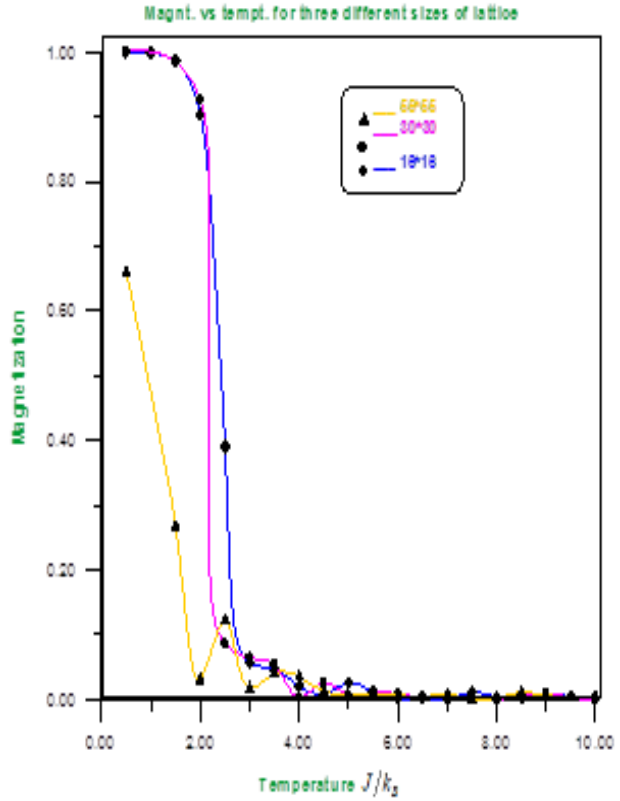

Figure 5: Magnetization against the temperature for three different sizes of lattice for case of zero external field (B=0).

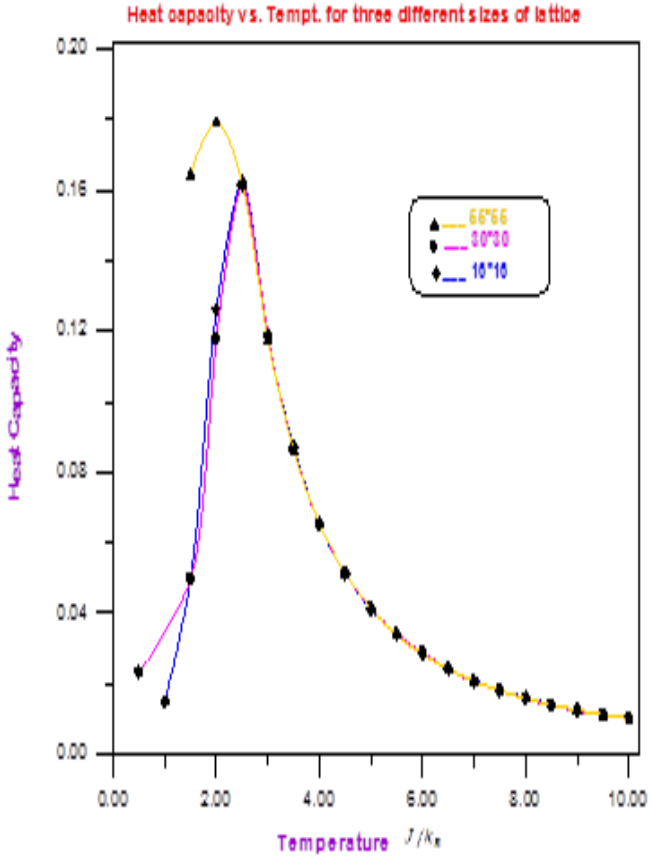

Figure 6: Heat capacity (in J -unity) against the temperature for different sizes for case of zero external field (B=0) .

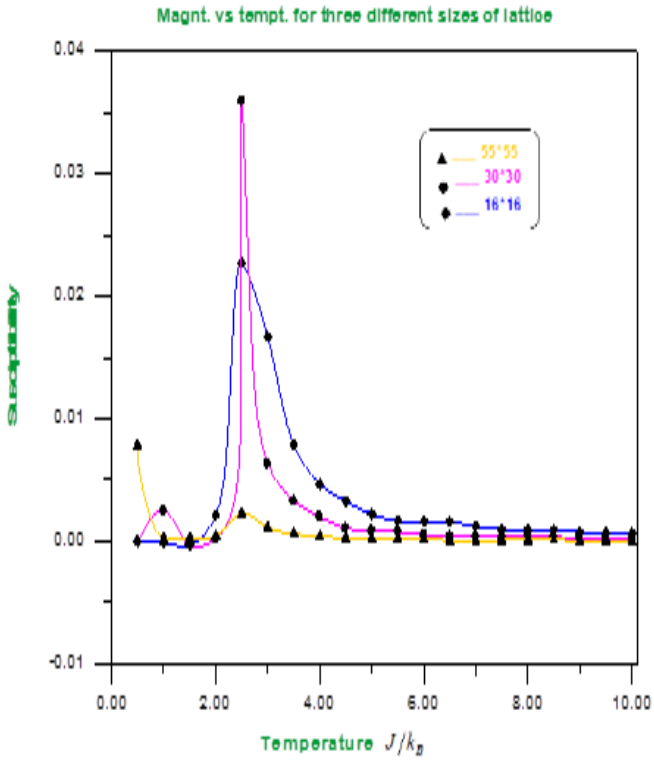

Figure 7: Susceptibility against the temperature for different sizes for case of zero external field (B=0) .

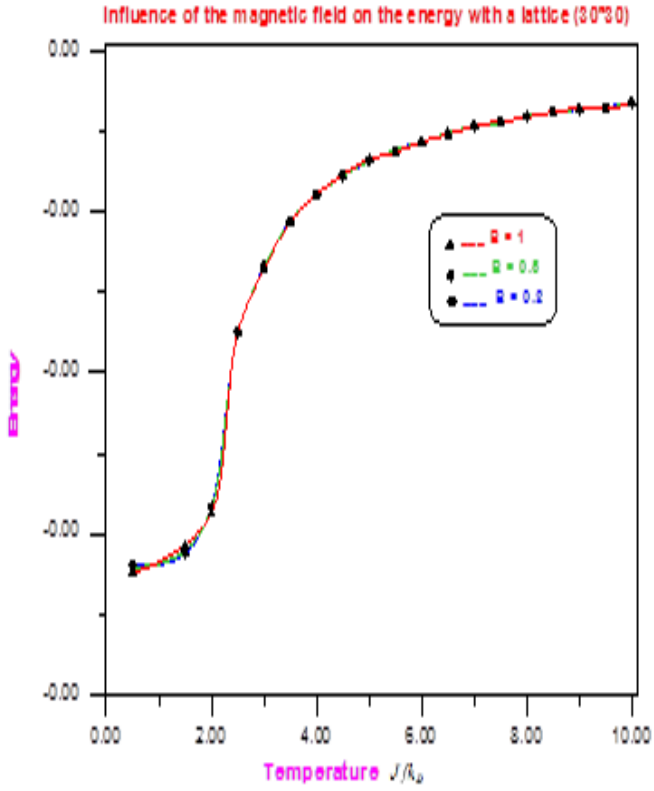

Figure 8: The influence of the external magnetic field on the energy on a lattice (30×30).

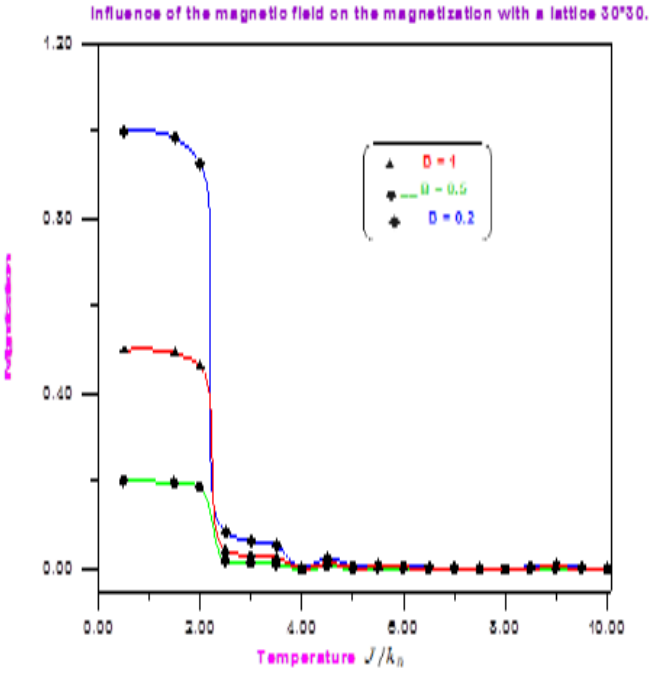

Figure 9: The influence of the external magnetic field on the magnetization on a lattice (30×30).

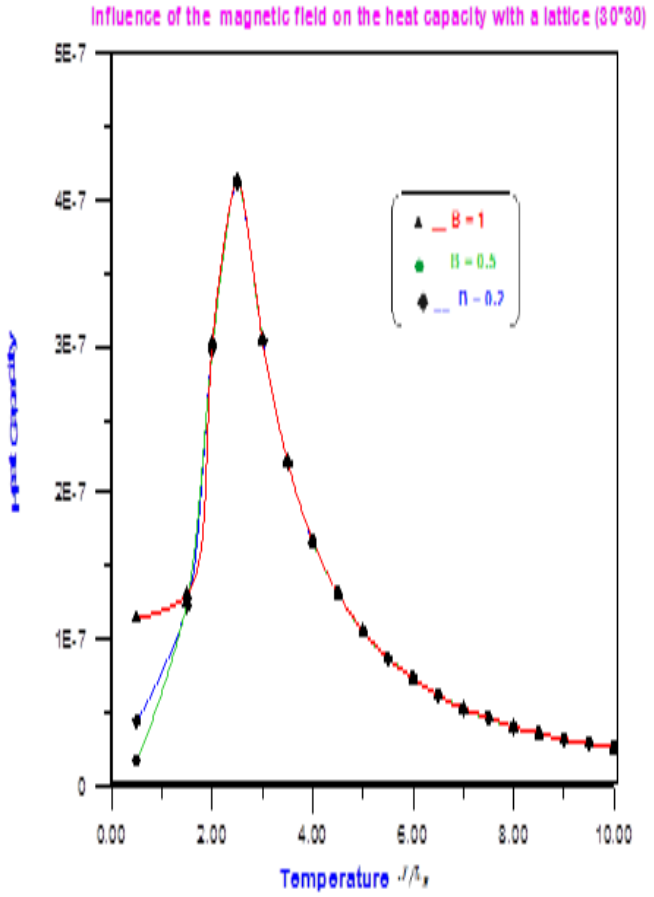

Figure10 : The Influence of the magnetic field on the heat capacity with a lattice (30×30).

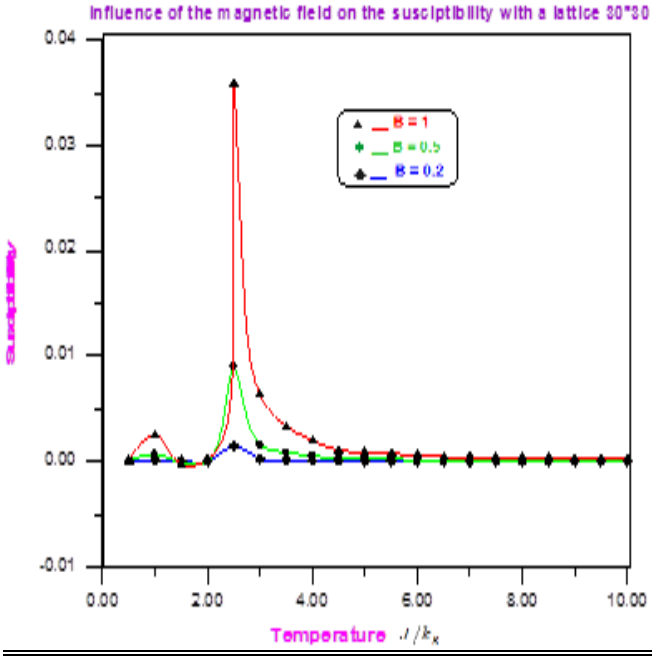

Figure11 : The Influence of the magnetic field on the susceptibility with a lattice (30×30).

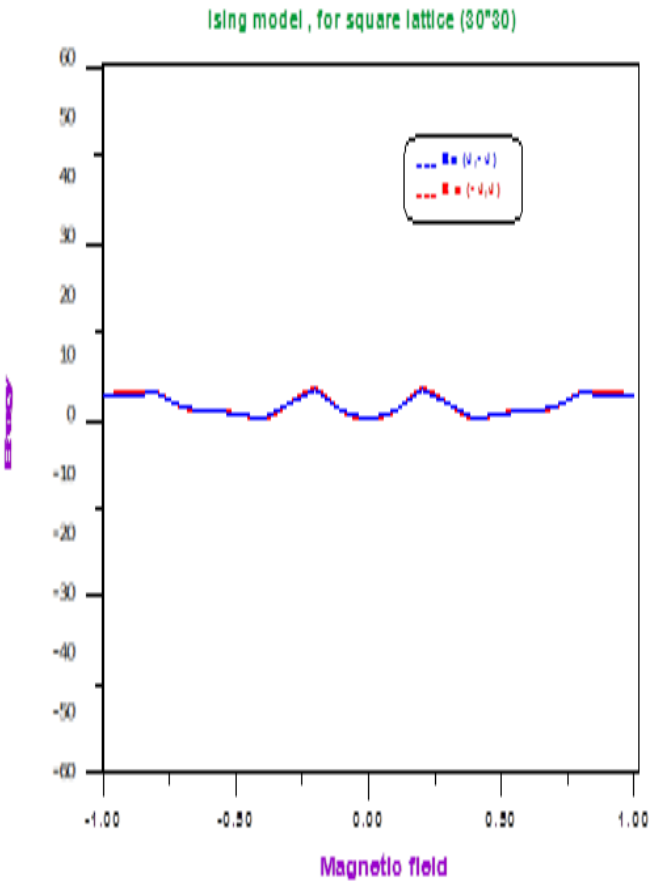

Figure 12 : $(\beta=0)$. Energy against the magnetic field with a lattice (30×30).

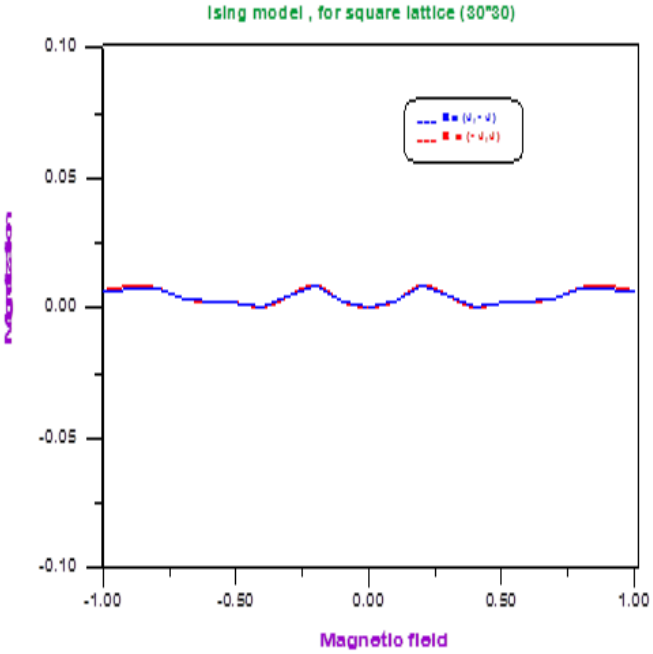

Figure 13 : $(\beta = 0)$ **. Magnetization against the magnetic field with a lattice** (30×30)**.**

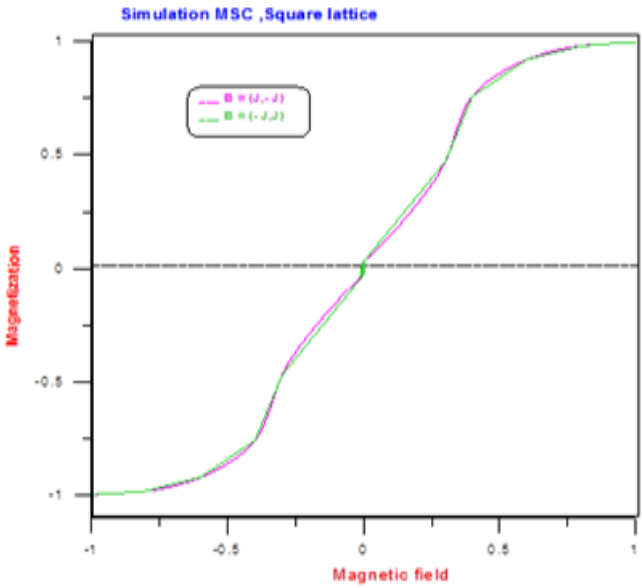

Figure 15 : $(\beta = 0.4)$ **. Magnetization against the magnetic field with a lattice** (30×30)**.**

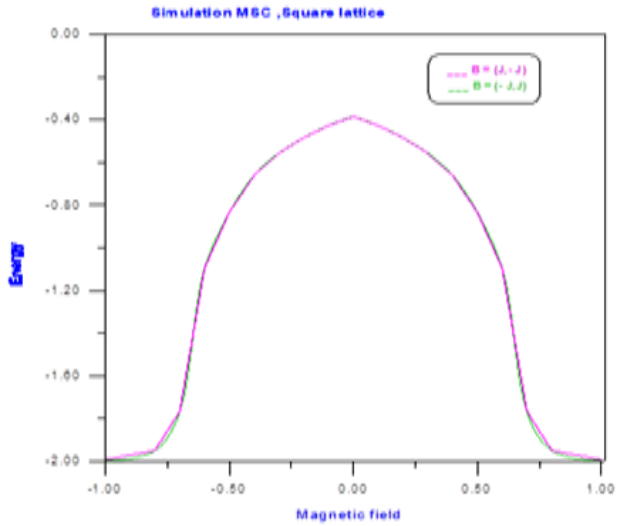

Figure 14 : $(\beta = 0.4)$ **. Energy against the magnetic field with a lattice** (30×30)**.**

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تطبيق نموذج Ising ثنائي الابعاد بطريقة مونتي كارلو

ضياء خالد خضير نبيل ابراهيم فواز

E.mail:

الخلاصة

تم تعيين موقع الانتقال الطوري ثنائي البعد لنموذج (Ising) بمعرفة درجة حرارة تدعى بدرجة حرارة كوري باستعمال محاكاة المونتي كارلو لمادة فيرومغناطيسية. وان المغناطيسية المكتسبة (M) لكل موقع للذرات (μ) ، الطاقة المكتسبة (E) لكل موقع (J) ، القابلية المغناطيسية (χ) ، السعة الحرارية (C_V) ، حسبت كدالة لدرجة الحرارة T لمصفوفة من تفاعلات شبيكة ذرات البرم $(16 \times 16 , 30 \times 30 , 55 \times 55)$ في مجال مغناطيسي $(B = 0, B \neq 0)$. استخدمت طريقة مونتي كارلو لتدقيق هذه النتائج ولتثبيت الانتقال الطوري. بينت نتائج التفاعل الداخلي (التلقائي) للبروم عند $(B = 0)$ انها متوافقة مع الحسابات النظرية لهذه الطريقة. اما عند مجال مغناطيسي $(B \neq 0)$ فان البروم تميل للاصطفاف مع المجال المسلط في حالة $(T > T_C)$ ، حيث ان تأثيره لم يكن فعال بدرجات الحرارة العالية بسبب التهيج الحراري الذي يعرقل اصطفاف البروم. وعند $(T < T_C)$ فهناك امكانية لاصطفاف البروم فقط اذا كانت قيمة المجال كبيرة.