Two Dimensional Ising Model Estimation With Monte Carlo Method For Different Lattice Sizes

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الخلاصة

تأثيرات حجمِ المشبّكِ على الانتقال الطوري ثنائي البعد لنموذج (Ising) حددت بإستعمال محاكاةِ مونتي كارلو لمواد فيرو مغناطيسية . وان **المغناطيسية** المكتسبة لكل موقع للذرات (μ) ،**الطاقة** المكتسبة لكل موقع (j) ، حسبت كدالة لقوة التفاعل J لمصفوفة من تفاعلات شبيكة ذرات البرم $(22\times 22,98\times 98)$ في مجال مغناطيسي $(B=0)$. تبين نَتائِجَ أعمال المحاكاة بالحاسوبِ التُوافقُ مع مصادرَ أخرى تعرف بالقيمة الحرجةَ لقوّةِ التفاعلِ والقريبة من القيمة $(J_C=0.48)$ في صفر مجال مغناطيسي . أيضاً النَتائِج كَانتْ متّسقة مع قِيَمِ مونتي كارلو المتوقّعة النموذجية والنظرية للمشبّكِ الأكبر ذو تأثيرِ الحجمِ اللانهائي. كما تم دراسة تقدم (حركة) الكميات الديناميكية الحرارية وقوة التفاعلَ قُرْب الانتقال(J_C) وكذلك العلاقة بين الطاقةِ والمغناطيسية.

ABSTRACT

In this project, the effects of the size of the lattice on the transition of the Phase in the two dimensional ising model were determined by using Monte Carlo simulation. The ***magnetization*** per site $[\mu]$, the ***energy*** per site $[j]$ of a ferromagnetic materials were Calculated as a function of interaction strength (J) for $(22\times 22,\ 98\times 98)$ spin lattice interaction by using Monte Carlo Simulation of the 2D ising model in which the results of computer simulations agree with other sources that claim that the critical value of interaction strength is close to $(J_C=0.48)$, in zero magnetic field. Also the results were consistent with the expected Monte Carlo model and theoretical values for the bigger lattice in which infinite size effect. Further the evolution of the thermodynamic quantities and interaction strength near the transition as well the relation between energy, magnetization were examined.

INTRODUCTION

It is well known that the interplay between the competing interactions in many magnetic and superconducting materials as well as in complex systems leads to a rich phase diagram with a large number of phases and non-trivial types of ordering. As a vivid example of such systems, we investigate here the two-dimensional $(2D)$ ising model with competing ferromagnetic nearest-neighbor (S_i) and diagonal (S_j`) interactions on a square lattice L^2 [1].

Consider the two-dimensional ising model which has many appliances in condensed matter physics and field theory. Generally, ising models have degrees of freedom residing on a lattice which interact locally. Here, thermodynamic properties of a magnetic material are calculated using the metropolis algorithm. The degrees of freedom are spins of atoms interacting with each other and an external magnetic field [2]. The Ising model considered is a square lattice of spin sites with periodic boundary conditions, ranging in size from (22×22) to (98×98) with the standard Hamiltonian. The coupling constant J and the Boltzmann constant K_B are both set to 1 . Spin sites are assigned a value of ± 1 to

represent spin up and down respectively. Thus, the total magnetization *M* is simply the integer sum of all lattice spin sites, and the total energy *E* is defined as minus the coupling constant J times all the neighboring spin pairs that are aligned [3]. Ferromagnetism and antiferromagnetism are exchange interactions that are caused by Pauli's Principle and Coulomb interactions. If we consider two spins S_i and S_j, the exchange interaction is in the form of $(\pm J . S_i S_j)$, where J is a positive and distance-dependent coupling constant. This coupling constant is determined by the overlap that consists of Coulomb interactions [4].

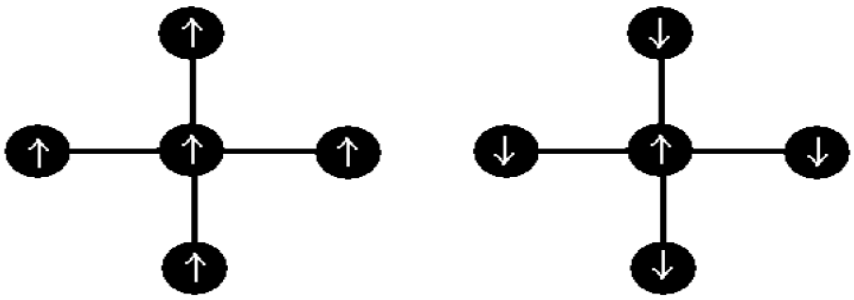

Figure-1: The energy of particle on the left is low since all the neighboring particles have the same alignment of spin. In contrast, the energy of the particle on the right is at its highest since all the neighboring particles have a different spin alignment [3].

THE MODEL AND METHOD

The Model

The particular model is a $n_i \times n_j$ square lattice with spin variables S. These can take two different values, $S_\alpha = S_{ij} = \pm 1 \; (\alpha = (i, j))$ which represents the either "`up"' or "`down"' state. The Hamiltonian for this system is [2]

$$H = -J \sum_{neighbours} S_\alpha S_\beta - B \sum_{\alpha} S_\alpha \qquad (1)$$

"Neighbors" means summation over the nearest-neighbor pairs of spins, i.e. spin $S_{i,j}$ interacts with the four spins $S_{i\mp1,\,j}$ and Periodic boundary conditions are assumed, so the upmost spin interacts $S_{i,\,j\mp1}$ also with the lowest, and the leftmost with the most right. We will be 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. We refer to figure (1) for better understanding of the proposed system.

The coupling strength is J; its sign defines the preferred spin orientation to minimize the total energy. This corresponds to ferromagnetic behavior. If J is positive, the energy minimum is achieved by orienting as many spins as possible parallel to each other. The orientation can be influenced by the external magnetic field B [2]. In order to compute the thermodynamics of this system, J and B can be measured in units of temperature. The system is configured by setting each spin variable, resulting in $2^{n_i . n_j}$ possible configurations S. The weighting of any one of these configurations in the canonical ensemble is therefore [2]:

$$w(S) = \frac{e^{-H(S)}}{Z} \tag{2}$$

with partition function

$$Z(J, B) = \sum_S e^{-H(S)} \tag{3}$$

The thermodynamic quantities which can be calculated are the energy E, the magnetization M, the susceptibility X and the specific Heat at a constant field C_B [2-5]:

$$E = \sum_S w(S)\, H(S) \tag{4}$$

$$M = \frac{\partial \log}{\partial B} = \sum_S w(S) \left(\sum_\alpha S_\alpha \right) \tag{5}$$

$$x = \frac{\partial M}{\partial B} = \sum_S w(S) \left(\sum_\alpha S_\alpha \right)^2 - M^2 \tag{6}$$

$$C_B = \sum_S w(S)\, H^2(S) - E^2 \tag{7}$$

Onsager [2,6] solved the ising model exactly in the limit of $n_i, n_j \to \infty$. For $B = 0$, the energy and magnetization then simplify to [2,6,7] .

$$E = -\left(n_i . n_j\right) J \coth(2J) \left(1 + \frac{2}{\pi} \kappa' K_1(\kappa) \right) \tag{8}$$

$$M = \pm \left(n_i . n_j\right) \frac{\left(1+z^2\right)^{\frac{1}{4}} \left(1-6z^2+z^4\right)^{\frac{1}{8}}}{\left(1-z^2\right)^{\frac{1}{2}}} \tag{9}$$

The specific heat is

$$C_B = \left(n_i . n_j\right)^2 \frac{2}{\pi} \left(J \coth(2J)\right)^2 \left(2K_1(\kappa) - 2E_1(\kappa) - (1-\kappa') \left(\frac{\pi}{2} + \kappa' K_1(\kappa) \right) \right) \tag{10}$$

Following short-hands are used in these expressions:

$$\kappa = 2\frac{\sinh\left(2J\right)}{\cosh^{2}\left(2J\right)} \tag{11}$$

$$\kappa' = 2\tanh^{2}\left(2J\right) - 1, \tag{12}$$

$$z = e^{-2J}$$

$$K_1(\kappa) = \int_0^{\frac{\pi}{2}} \frac{d\phi}{\left(1-\kappa^2\sin^2(\phi)\right)^{\frac{1}{2}}} \tag{13}$$

$$E_1(\kappa) = \int_0^{\frac{\pi}{2}} d\phi \left(1-\kappa^2\sin^2(\phi)\right)^{\frac{1}{2}} \tag{14}$$

There is a critical value $(J_C = 0.4868)$ for which $k = 1$, where K_1 has a logarithmic singularity. Therefore, all thermodynamic functions are singular at J_c, which corresponds to a phase transition. Here, the magnetization vanishes for couplings lower than J_c. Stronger couplings result in a magnetization taking on one of two equal and opposite values.

Monte Carlo Simulation Method

The $N^2 - array$ is initialized at a low temperature with aligned spins or at a high temperature with random values (1 or −1). Then, the evolution at a given temperature is achieved by following the Metropolis algorithm which ensures a Boltzmann distribution, i.e the probability that the system is in the S configuration is given by using equations (2,3) [4-8]:

$$w\left(S\right) = \frac{e^{-H(S)}}{Z}$$

$$Z(J,B) = \sum_{S} e^{-H(S)}$$

The Monte Carlo method consists to choose randomly a spin to flip. The chosen spin is flipped if it is favorable for the energy. The system has 2^{N^2} configuration, the Metropolis algorithm allows not to test each configuration to reach the equilibrium. The Boltzmann distribution maximizes the entropy, so it reduces the free energy.

When the energy becomes stable, the system reached the thermalisation. Then, several configurations are determined by the Metropolis algorithm in order to determine the properties of interest as the energy and magnetization for types from lattices. In presence of magnetic field: the spins align with the magnetic field.

- 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.
- 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) [8] . 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.

RESULTS AND DISCUSSION

Influence of the size of the lattice on the characteristic quantities *:* Smaller lattice

In order to see the effect of the size of the lattice on the transition of the phase, the interaction strength is plotted for lattice size (22×22) in the absence of magnetic field . begin by creating a square lattice with $(22\times 22=484)$particles and assign random spin orientation. Choose a random value between $(0\ and\ 1)$ for the interaction strength and then watch how the system evolves over (900) steps to reach an equilibrium. The effect of interaction strength for this lattice on energy and magnetization have been shown in figures (2,3) . Also, the magnetization per site as a function of energy is shown in the figure (4).

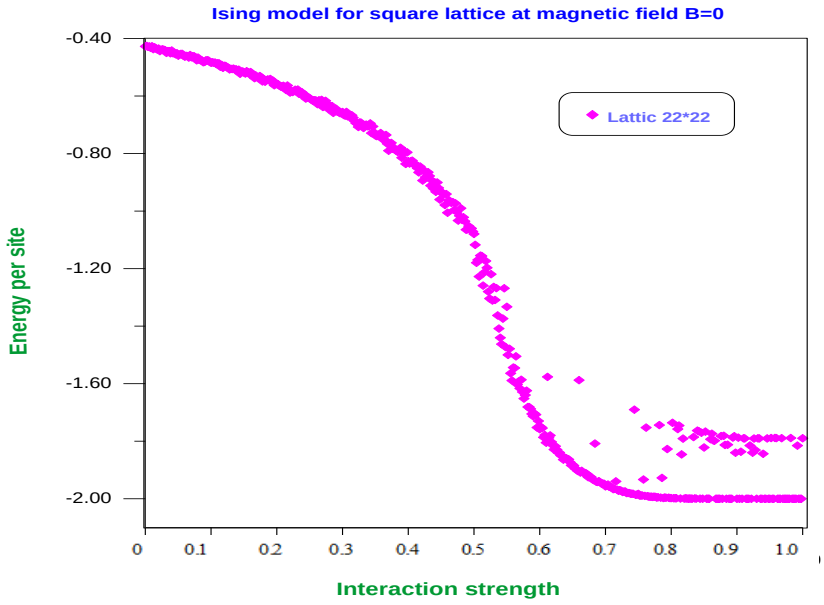

Figure-2: Energy as a function of interaction strength for the (22^2) particle lattice

In figure (2) one can see the speed of evolution is controlled by the variable or (value J = 0.2) .Value of (0.2) means that only 20% percent of the originally selected group will have its spin flipped. In essence this parameter tries to mimic the evolution of real systems. Even though a certain particle will have a smaller energy with its spin flipped it doesn't mean that all particles in the lattice that follow that criterion will have their spins flipped immediately. Although the total energy of the system as function of interaction isn't very distinctive one can see some transition at an interaction strength between (0.5 and 0.55). This can be seen more clearly when one look at the change in magnetization as a function of interaction strength, see figure 3.

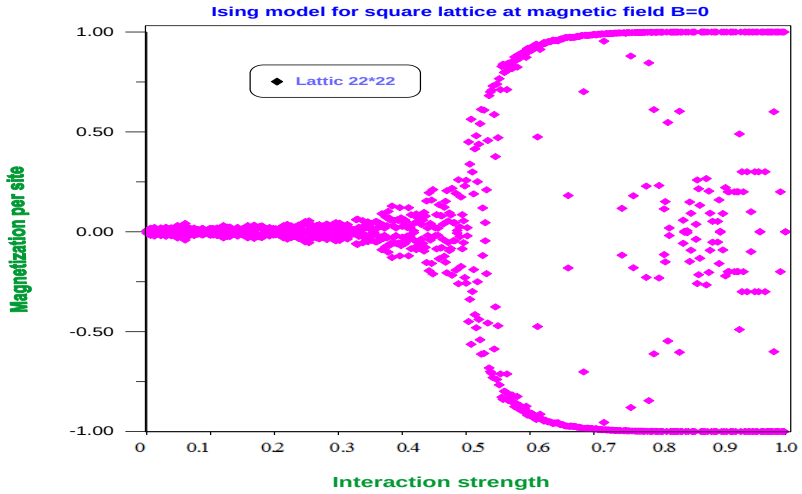

Figure- 3: Magnetization as a function of interaction strength for the (22^2) particle lattice.

At higher interaction strength , the system strongly favors the two ground states. These are states with all spins aligned, either all up $(M=1)$ or all down $(M=-1)$. At strength of interaction slower than the phase transition, the spins tend to be randomly aligned, which results in $(M=0)$. This corresponds to a high temperature (the crossing of Curie's temperature) since $(J=-E/kT)$which means that (J) is inversely proportional to T . However, as we increase the interaction strength the spins tend to align.

The relation between magnetization and energy for lattice (22×22) have been shown in figure (4) .

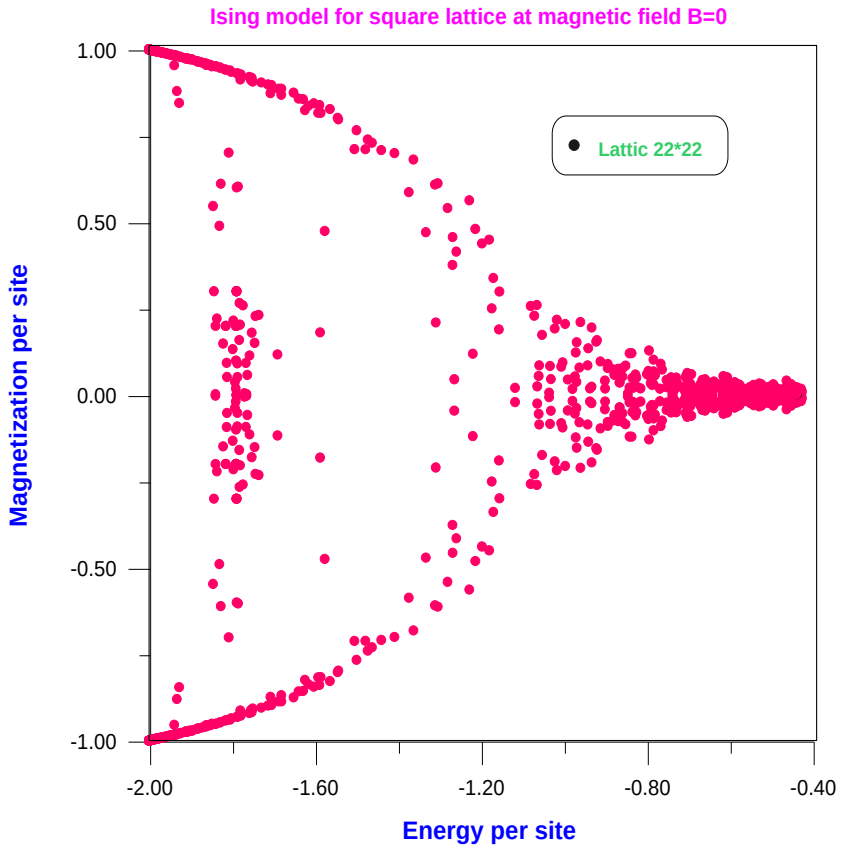

Figure- 4: Magnetization as function of energy for the (22^2) particle lattice.

There are two regions of low energy corresponding to spin up orientation and spin down. There are also low energy cases that do not show a high net Magnetization. This happens when relatively large clusters of either spin up and spin down. This is analogous to the domains of ferromagnets. It is good to notice that a net Magnetization or the formation of domains leads to decreased energy.

Influence of the size of the lattice on the characteristic quantities :

A bigger lattice

The influence of the lattice size clearly visible when the phase transition at an interaction strength $(J = 0.6)$ for lattice with higher number of particles in the absence magnetic field. We notice that if the size is big enough, the phase transition is really perceptible. The effect of interaction strength for (98×98) lattice on energy and magnetization have been shown in figures (5,6) . Also the magnetization per site as function of energy is shown in the figure (7) .

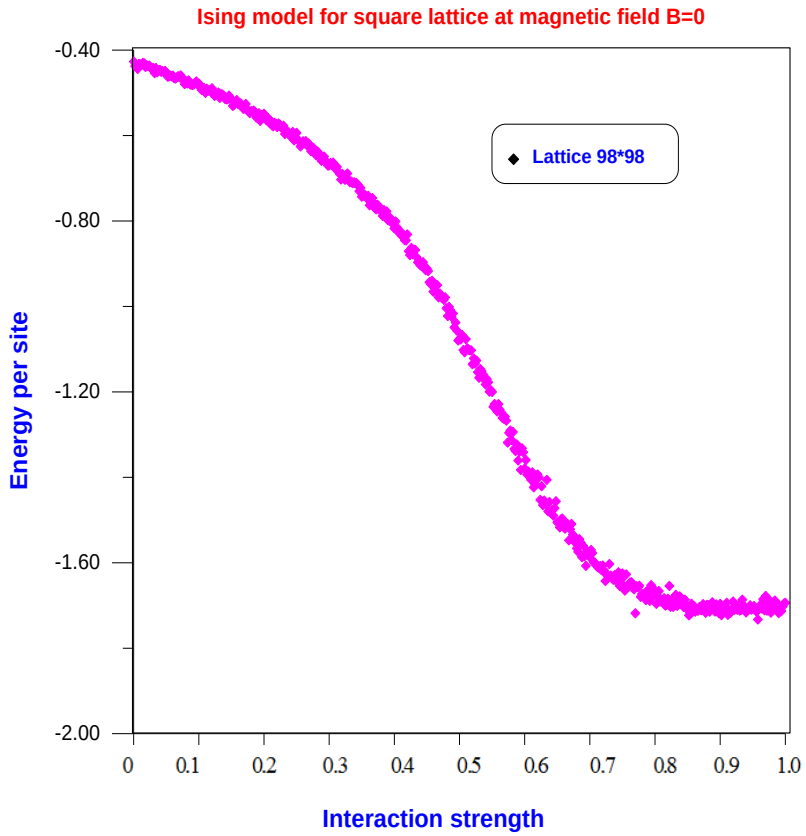

Figure- 5: Energy as a function of interaction strength for the (98^2) particle lattice.

In figure (5) the phase transition is much more apparent. Initialize a square lattice with (98^2) particles and watch how the system evolves over $((98 \times 98)=9604)$ steps to reach an equilibrium.

The splitting of the line which becomes more apparent as interaction strength increases is probably due to different energy for the lattice with domains, i.e. zero net magnetization, and the lattice with a total magnetization of $(-1 \; or \; 1)$ [4].

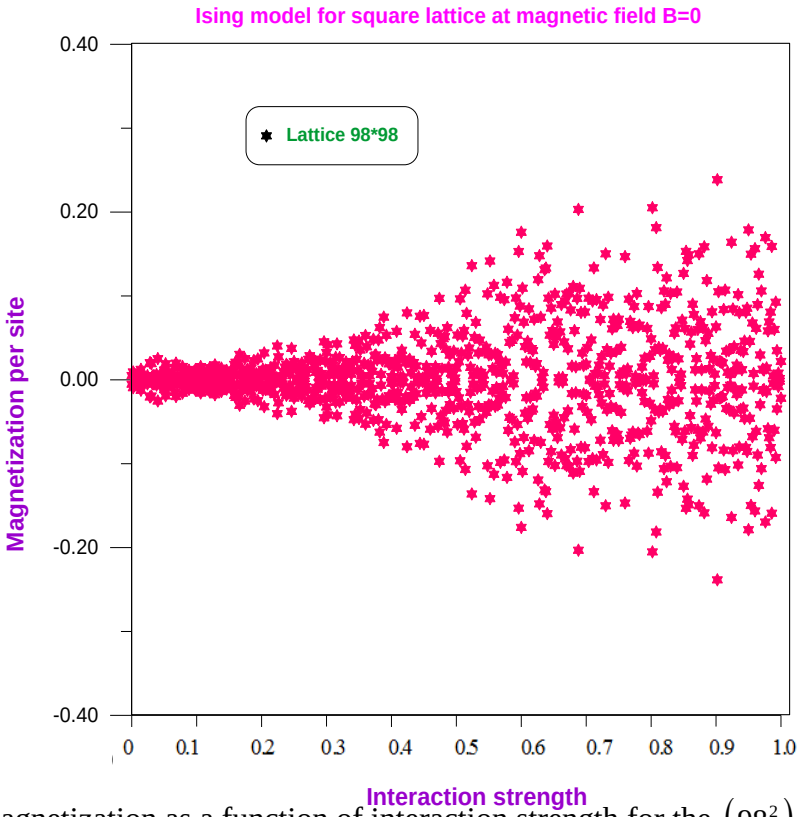

Figure- 6: Magnetization as a function of interaction strength for the (98^2) particle lattice.

In figures (6 and 7) the population of atoms in case of $(22\times 22 = 484)$ are more distinguishable for $(M = 1)$ and $(M = -1)$ branches than (98×98) for the case of a particle lattice. It turns out that this is in agreement with theory. We will end by comparing these results with theoretical model .

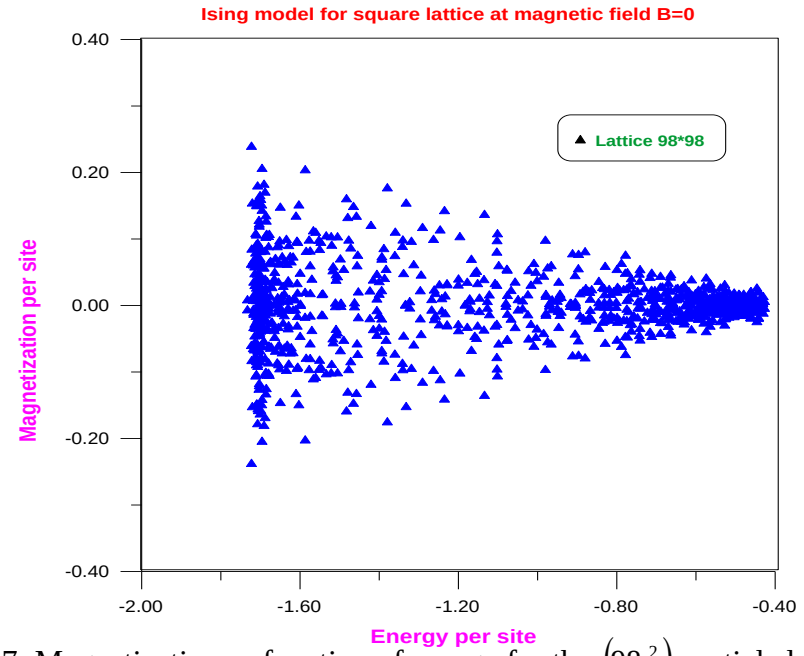

Figure- 7: Magnetization as function of energy for the (98^2) particle lattice.

In figure (7) at high interaction strength there appears to be also a class of 'metastable' states in which approximately half of the spins are up and approximately half are down, with aligned spins forming large contiguous clusters.
These states account for the cluster of points around $(M=0)$ at high interaction strength, and, therefore, the lower of the two lines in the energy plot (as the boundary between the spin-up cluster and the spin-down cluster will decrease the energy slightly from the ground state).
It is also interesting to plot magnetization versus energy, which is done in figure (7). Higher-density regions indicate the four states. Around $(M=\pm 0.4\,,\ E=-2)$ we find the two high interaction strength ground states; centered at $(M=0\,,\ E=-0.7)$ we find the low interaction strength phase; and around $(M=0\,,\ E=-1.7)$ we find the high interaction strength metastable states.

Comparing the Model with theory

It is easy to calculate the theoretical values for energy and magnetization according to equations (8) and (9) by using analytical solutions methods. One can see compare between the results Monte Carlo model and theoretical values for the bigger lattice (98×98) have been shown in figures (8,9) . The theoretical model assumes an infinite lattice which affects the meaning of all comparisons. It is however a reassuring thing that Monte Carlo model gives better results for the bigger lattice. One can see that the theoretical model for the energy is quite different from what obtain using model, see figure 8.

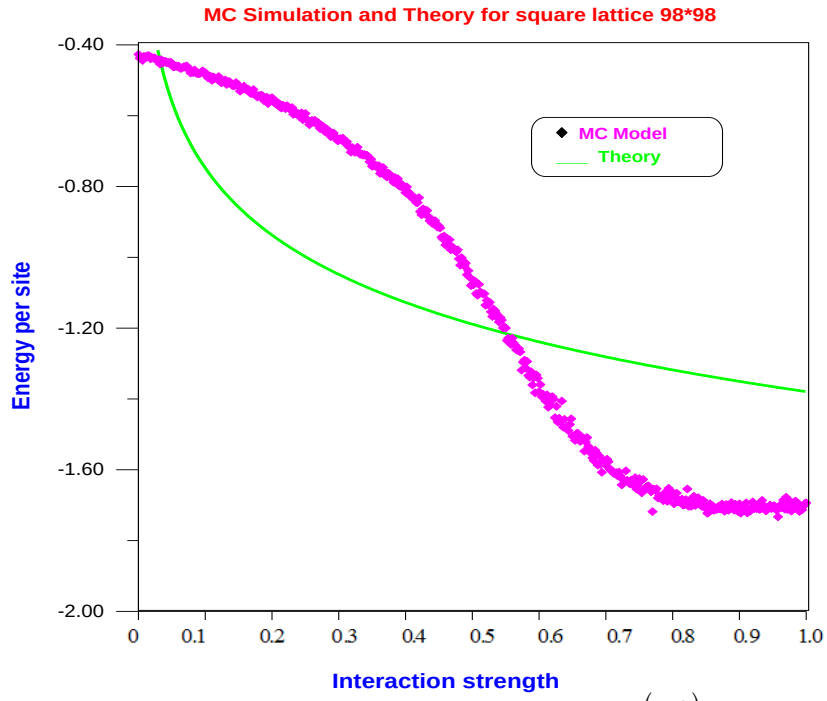

Figure -8: Energy as a function of interaction strength for the (98^2) particle lattice.

According to theory the energy per site goes to infinity when the interaction strength goes to zero. This is in agreement with the fact that the interaction strength is reversely proportional to temperature and as temperature goes to infinity the energy of each particle should too.

In figure (9) one see a much nicer agreement between theory and the Monte Carlo model.

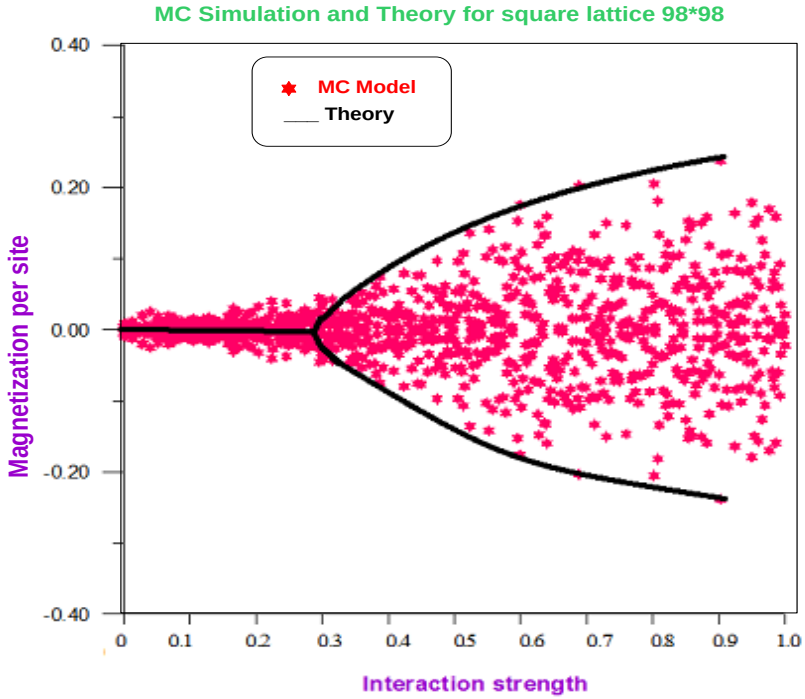

Figure- 9: Magnetization as a function of interaction strength for the (98^2) particle lattice.

There are high interaction strength cases where the net magnetization is close to zero and these correspond to the formation of domains in ferromagnetic materials [4].

CONCULOSIONS

The Monte Carlo method applied to the ising model which describes the magnetic properties of materials allows to obtain the thermodynamic quantities variations with different lattice sizes. The results were consistent with the expected Monte Carlo model and theoretical values for the bigger lattice in which infinite size effect. All the values calculated, based on the fact, that the only positive coupling constant (interaction strength) are used . In this case one can see that the exchange energy, $((-J.S_1 S_2))$, is negative and thus the spins prefer to be parallel, which leads to ferromagnetism. Hence, below the $(J = 0.5 - 0.6)$, becomes spontaneous magnetization.

in the case of the bigger lattice, to reach an equilibrium, the evolution of the system over $(98 \times 98 = 9604)$steps only is needed .

There are two reasons for an increased computational time in a larger lattice.

1- Since it is bigger the flipping of spins for more particles needs to be decided.

2- It takes greater time for a larger system to reach equilibrium which that must be let the system evolve over a larger number of steps. In this case, since the calculations are more demanding.

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