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2D-Ising model for Simulation of Critical Phenomena of $NiOFe_2O_3$ using Monte Carlo Technique

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ABSTRACT: In this work, the critical phenomena of Nickel II Iron III oxide (Ferromagnetic) shall be determined using Monte Carlo simulation technique. The critical temperature (T_c), the magnetization per site (μ), energy per site (E), magnetic susceptibility (χ), specific heat of a $NiOFe_2O_3$ are determined as a function of temperature for two different square lattices 20x20 and 150x150. The analysis of simulation results indicates that the bipolar magnet with strong tetragonal distortion in external magnetic field applied along the axis resembles the behaviour of the two dimensional Ising model on the rectangular lattices. The numerical solution of the model in MATLAB "R2013a" is presented. For the sake of clarity, a Monte Carlo Algorithm known as Metropolis Hastings Algorithm was used to evaluate the behaviour of the lattice and the critical temperature at which the phase transition between $NiOFe_2O_3$ and paramagnetic state occurs was noted. The analysis of the results shows that $T_c = 2.25J/K_B$, in the absence of external magnetic field. It was observed that above (T_c) the material ($NiOFe_2O_3$) becomes a paramagnetic state, and this leads to decreasing in average magnetization and the average Energy increases, while below (T_c) the material is in a ferromagnetic state.

KEYWORDS: Critical temperature, Ferromagnetic, Lattice, Simulation, Susceptibility, Nickel.

INTRODUCTION

One of the most interesting and outstanding problems in modern equilibrium statistical mechanics is the understanding of the physical and mathematical mechanisms of phase transitions. Virtually all substances in nature exhibit cooperatively in one sense or another, some substances display critical phenomena by undergoing a change of phase in configuration space at some critical temperature. Phase transition and critical phenomena are the most universal phenomena in nature. The square-lattice Ising model is the simplest system showing phase transitions (i.e. the transitions between the paramagnetic and ferromagnetic phase) and critical phenomena at finite temperatures. The square lattice Ising model has played a central role in the understanding of phase transitions and critical phenomena [1]. The exact solution of the square- lattice ising model with periodic conditions is well known both in the thermodynamic limit (that is, the infinite size system)[2] and finite size system. However, the exact solution of the square lattice ising model with free boundary conditions is not known for system of arbitrary size.

Analysis of dynamic critical properties is a major problem in statistical physics and theory of phase transition [3],[4]. The substantial progress achieved to date in this field became possible mainly through theoretical and experimental studies. Nevertheless, the development of a rigorous and consistent theory of dynamic critical phenomena based on microscopic Hamiltonians remains a challenging problem in the modern theory of phase transitions and critical phenomena [5],[6]. The critical dynamics of magnetically ordered crystals, especially Gadolinium (Ferromagnetic), is characterized by a great diversity and complexity due to the importance of both exchange interaction and relatively weak relativistic effects (such as anisotropy and dipole-dipole interaction). The most essential factor of the latter kind is dipole-dipole interaction, which plays an increasingly important role as the critical point is approached. Note that the aforementioned classification of universal dynamics critical behaviour does not allow for any effect due to dipole –dipole interaction. further analysis [7-9] have shown that theories taking into account dipole-dipole interaction predicts dynamics of two types, normal and stiff, each characterized by a specific set of critical exponents.

It is clear that experimental studies can hardly elucidate the current discrepancy between observations and predictions, because high-precision measurement of critical parameters is a very difficult task. Moreover, since almost any experimental result is due to the combined effects of all factors, their individual strengths and contributions are practically impossible to single out. The problem is also unlikely to be amenable to rigorous theoretical analyses in view of enormous mathematical difficulties.

In recent studies, method of computational physics has played an increasingly important role in dealing with complex issues of this kind. Highly accurate and reliable calculations of critical parameters can be performed by applying these methods, at least, in studies of static critical behaviour [10]. In particular, the advantages of Monte Carlo and molecular theory dynamics simulations include not only rigorous mathematical foundations and error control within their respective frameworks, but also the possibility of evaluating the relative importance of individual parameters.

The approach to ferromagnetism as a function of temperature is described by the Curie –Weiss law [10] which gives the magnetic susceptibility as a function of temperature

$$\chi = \mu - 1 = \frac{C}{T_C} \qquad (1)$$

Where χ *and* μ are the magnetic susceptibility and relative magnetic permeability of the material respectively, C is a constant and T_C is the curie or critical temperature. Equation (1) valid above the Curie temperature. The relative magnetic permeability of the sample can be written as

$$\mu = \frac{L(T)}{L_o} \qquad (2)$$

Where L(T) is the inductance of the coil at temperature T and L_o is the inductance of the coil without the sample. This is not exactly the relative permeability since not all the magnetic flux will couple to the sample. From equation (1) and (2)

$$\left(\frac{L(T)}{L_o} - 1\right)^{-1} = \frac{T - T_C}{C} \qquad (3)$$

The left hand side of equation (3) is zero when T = Tc.

Several works has been done on 2-D Ising model of feromagnetics by different scholars. Bhanot [11] computed the exact partition functions of the Ising model on L x L square lattices with free boundary conditions up to L = 10 using Cray XMP. Bhanot counted all $2^{L \times L} = 2^{100}$ ($\approx 1.27 \times 10^{30}$) states for L = 10, and began obtaining some useful results.

Stodolsky and Wosiek [12] obtained the exact partition function for L = 13 (corresponding to $2^{169} \approx 7.48 \times 10^{50}$ states) using IBM RISC 6000, and studied phase transitions based on the entropy as a function of the energy.

In this work, for the first time, we evaluate the exact partition function and simulate the critical phenomena of $NiOFe_2O_3$ on L x L square lattices with free boundary conditions for L = 20 and 150.

SIMULATION PROCEDURE

In this work, we consider a two dimensional square lattice of spins. In the absence of external magnetic field, the Hamiltonian of a spins system is written as:

$$H = j \sum_{(i,j)}^{N} \sigma_i \sigma_j \qquad (4)$$

Where J is the interaction energy of the two spins, N is the total number of spins [1] and σ_i *and* σ_j is the spin along x and y direction respectively.

we gradually increased the temperature (T) from absolute zero and at some value of T, the magnetization changes its state from high value to a low value (that is, phase transition occurs).

We have ran a number of Monte Carlo simulations for 20 x 20 square lattice $NiOFe_2O_3$ and plotted various graphs to determine critical temperature and critical point exponent of the square lattice used. Here it is assumed that only the nearest neighbors affect each spin (that is, in a 2D square lattice, each spin has four neighbours: up, down, left and right).

MEASUREMENT

Spontaneous magnetization and magnetic susceptibility was measured as follows: for the nth state per spin magnetization

$$m_n = \frac{1}{L^2}\sum_i^{L^2} \sigma_i{}^n \tag{5}$$

L is the size of the lattice that is 20 x 20, S_i is the i^{th} spin. The change in magnetization is given by

$$\Delta M = M_m - M_n = 2s_k{}^n \tag{6}$$

we calculated the magnetization at beginning of the simulation and then use the following equation

$$M_m = M_n + \Delta M = M_n + 2s_k{}^n \tag{7}$$

For every spin, as soon as the magnetization was obtained, we calculate the per spin susceptibility as

$$\chi = \frac{\partial \langle M \rangle}{\partial H} = \frac{\beta}{L^2}(\langle M^2 \rangle - \langle M \rangle^2) \tag{8}$$

or, $\chi = \beta(\langle M^2 \rangle - \langle M \rangle^2)$ (9)

where $\beta = \frac{1}{K_B T}$

Energy and specific heat were determined as shown below

$$E_n = -J\sum_{i,j} \sigma_i{}^n \sigma_j{}^n \tag{10}$$

We set the J = 1 and the energy difference in going from state n to m is determined

$$E_m = E_n + \Delta E \tag{11}$$

Knowing the value of E, we then calculated the specific heat per spin as

$$C_V = \frac{\beta^2}{L^2}(\langle E^2 \rangle - \langle E \rangle^2) \tag{12}$$

Taking $K_B = 1$

RESULTS

We have started with random spin at the lattice sites and calculated initial magnetization and energy using Ising model. We implemented Hasting Metropolis Monte Carlo simulation of an Ising model in Matlab. All the simulations were of 20 x 20 and 150 x150 square lattices of $NiOFe_2O_3$, we run for temperature of 0.0J/K_B through 5.0 J/K_B. After each temperature increment, the system was allowed to equilibrate for 15,000 steps, and then the averages were performed over the entire grid. The code for the programme is shown in appendix A. (we choose the strength of interaction as J=1 and set the Boltzmann's constant K=1, so temperature becomes dimensionless). in all the four plots, the phase transition from the $NiOFe_2O_3$, ferromagnetic state, where magnetization is maintained even though there is no external magnetic field, and the paramagnetic state, where the temperature is high enough to render the spin-interactions insignificant, it readily observable. Once the critical temperature is reached, the spins have enough energy to overcome the barrier to flipping.

In all plots, the phase transition from the ferromagnetic state, where magnetization is maintained even though there is no external magnetic field, and the paramagnetic state, where the temperature is high enough to render the spin-interactions insignificant, it readily observable. Once the critical temperature is reached, the spins have enough energy to overcome the barrier to flipping. Thus, the magnetization breaks down and oscillates about zero, since each spin is essentially equally likely to be spin up or down.

Further, the plots can be seen exhibit phase transitions right around 2.25J/K_B.

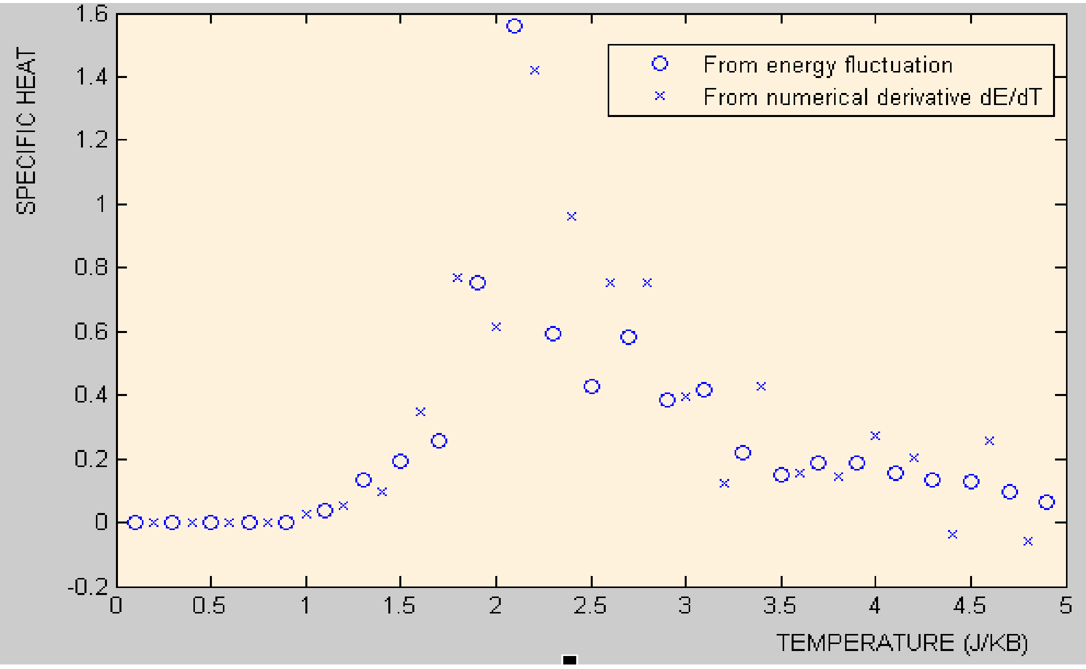

Figure 1: plot of specific heat C against temperature T (in the unit J/K_B) for 20x20 square lattices of $NiOFe_2O_3$

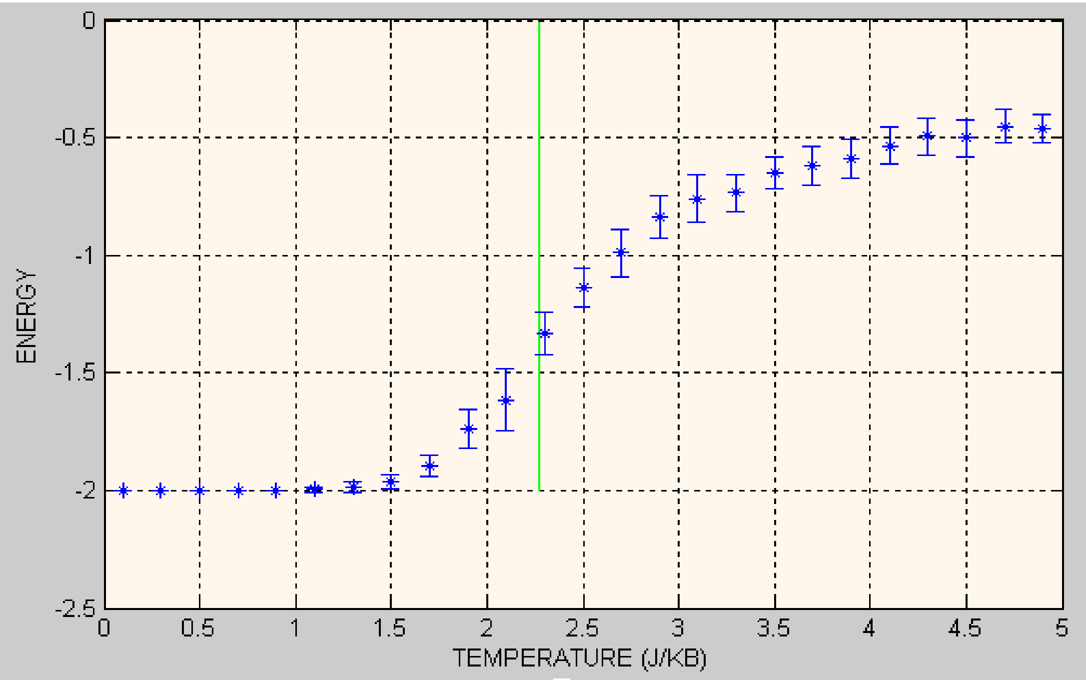

Figure 2: plot of Energy, E against temperature T (in the unit J/K_B) for 20x20 square lattices of $NiOFe_2O_3$

The green vertical line shows the location of the exact critical temperature Tc in the thermodynamical limit. J = 1, L = 20, and B = 0.

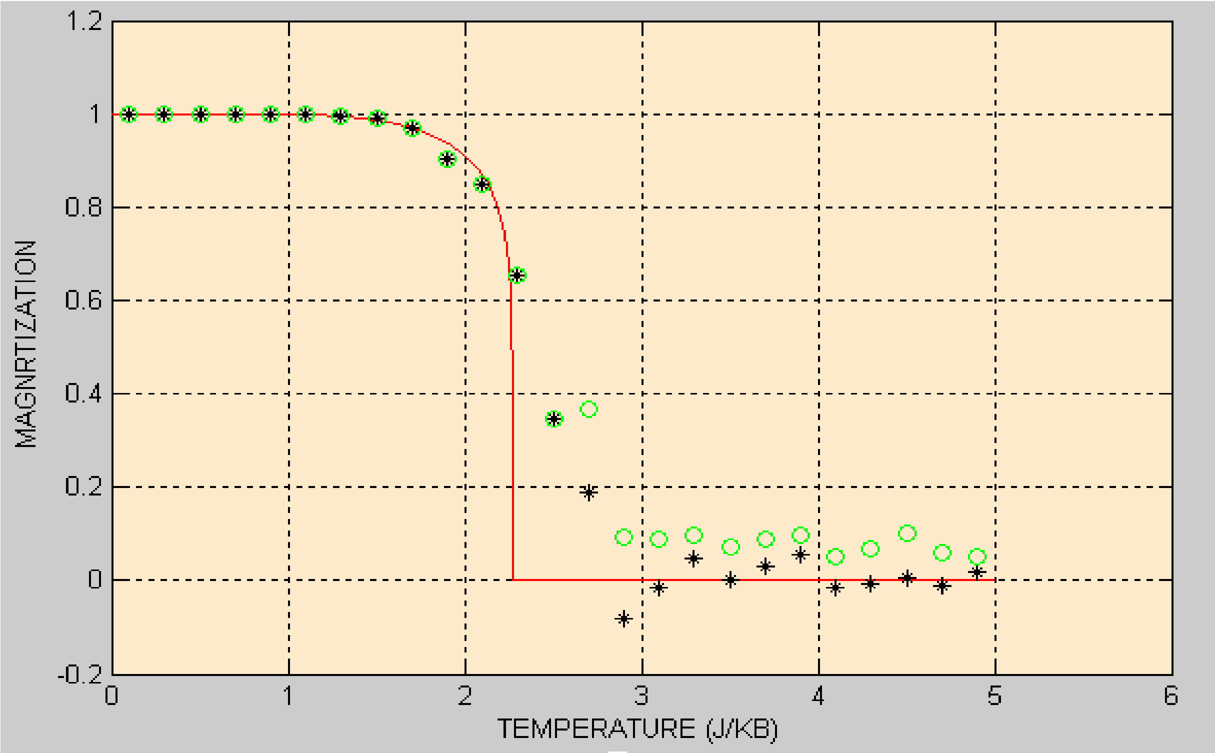

Figure 3: Average magnetization per site of a $NiOFe_2O_3$ as a function of temperature for 20x20 square lattices.

2D ising model magnetization compared with exact B=0 result in the thermo dynamical limit (red line, spin upside).

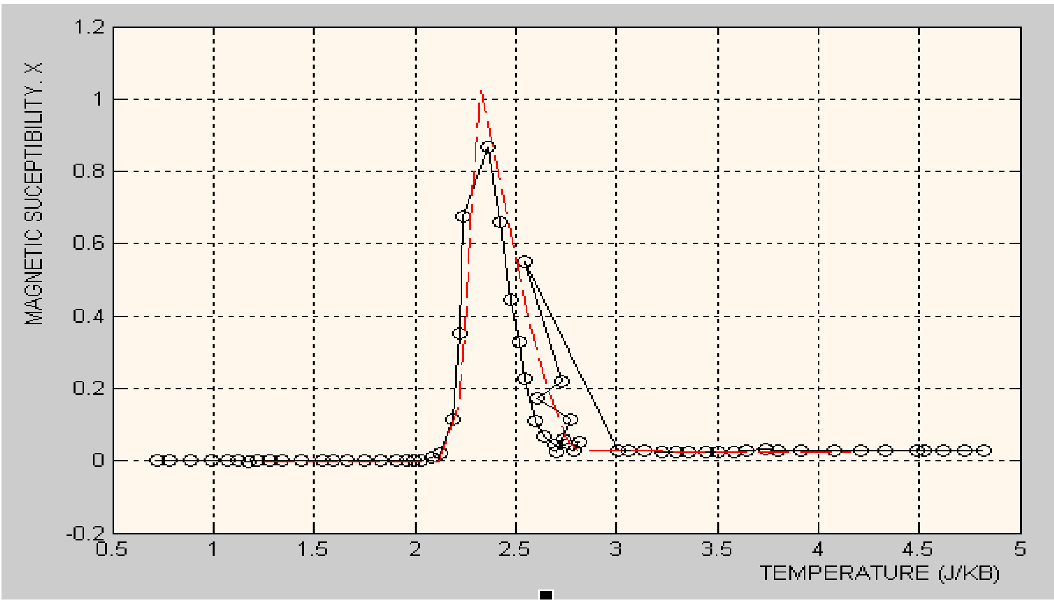

Figure 4: Magnetic susceptibility of a $NiOFe_2O_3$ as a function of temperature for 20x20 square lattices.

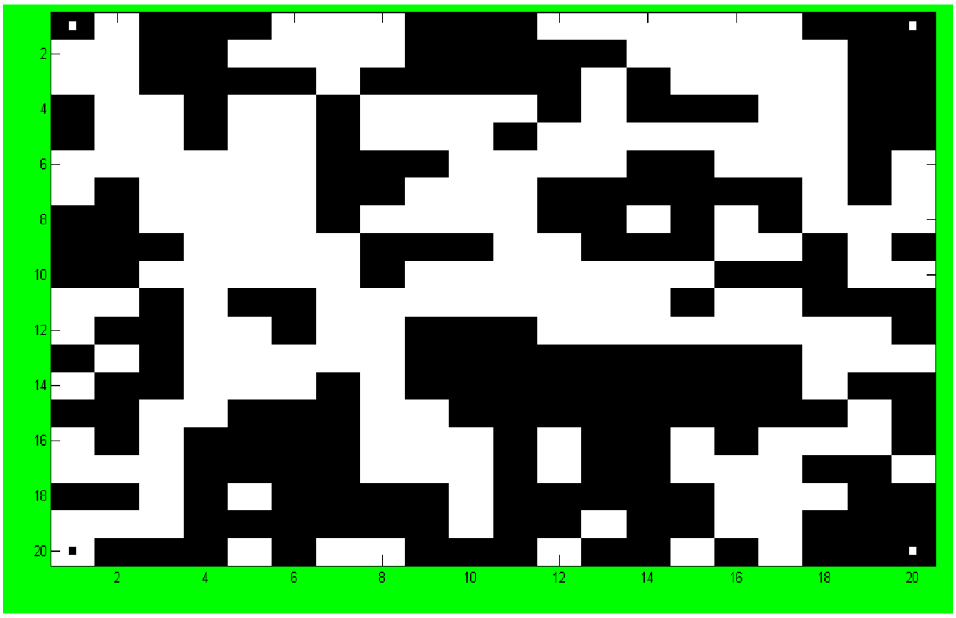

Figure 5: Equilibrium spin configuration at different temperatures around T_c after 15,000 steps for 20x20 square lattices.

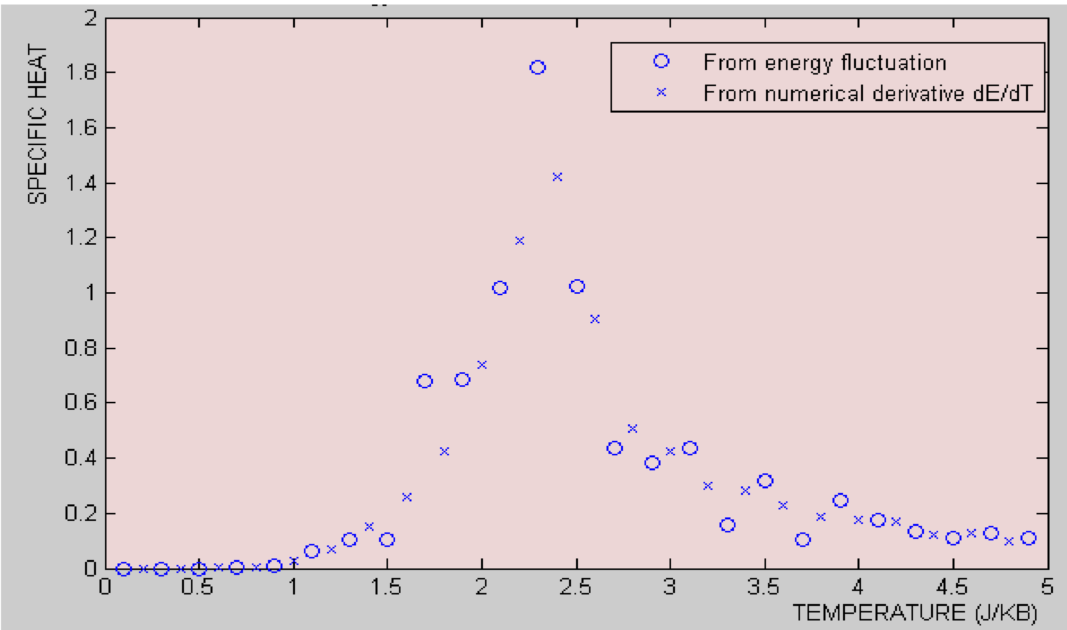

Figure 6: plot of specific heat C against temperature T (in the unit J/K_B) for 150x150 square lattices

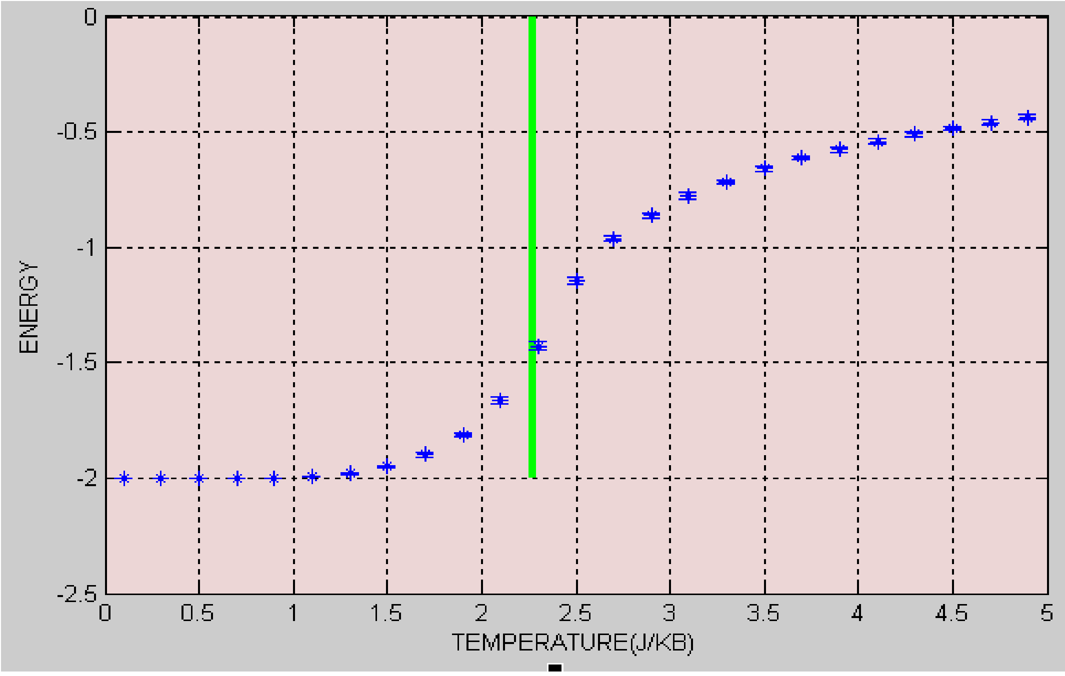

Figure 7: plot of Energy, E against temperature T (in the unit J/K_B) for 150x2150 square lattices $NiOFe_2O_3$

The green vertical line shows the location of the exact critical temperature Tc in the thermodynamical limit. J = 1, L = 20, and B = 0.

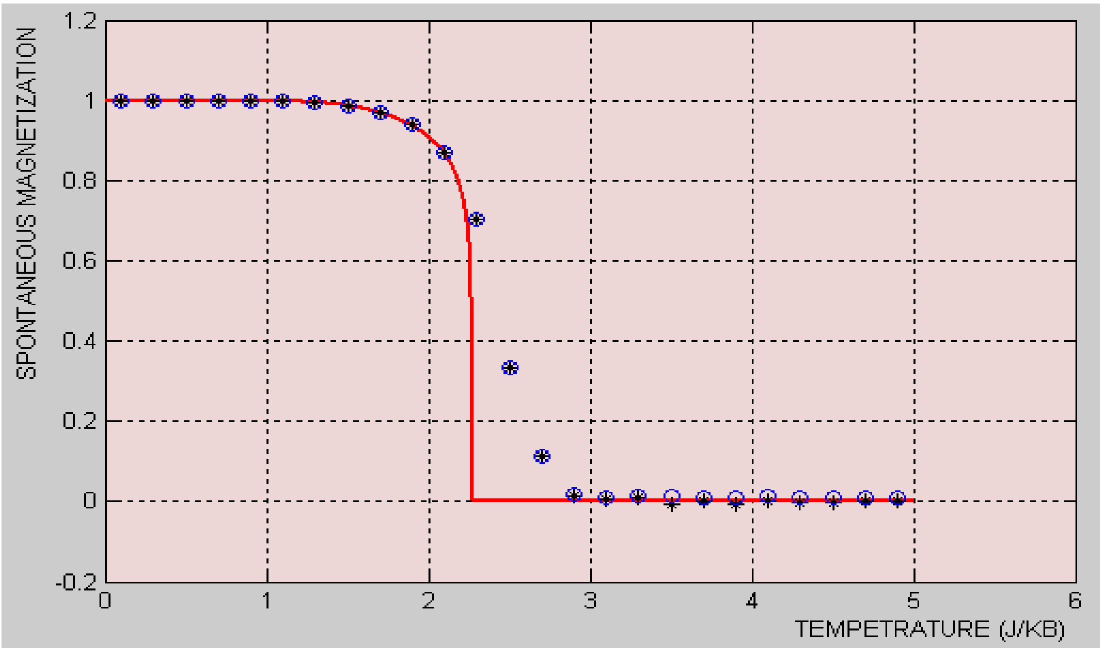

Figure 8: Average magnetization per site of a $NiOFe_2O_3$ as a function of temperature for 150x150 square lattices.

2D ising model magnetization compared with exact B=0 result in the thermodynamical limit (red line, spin upside).

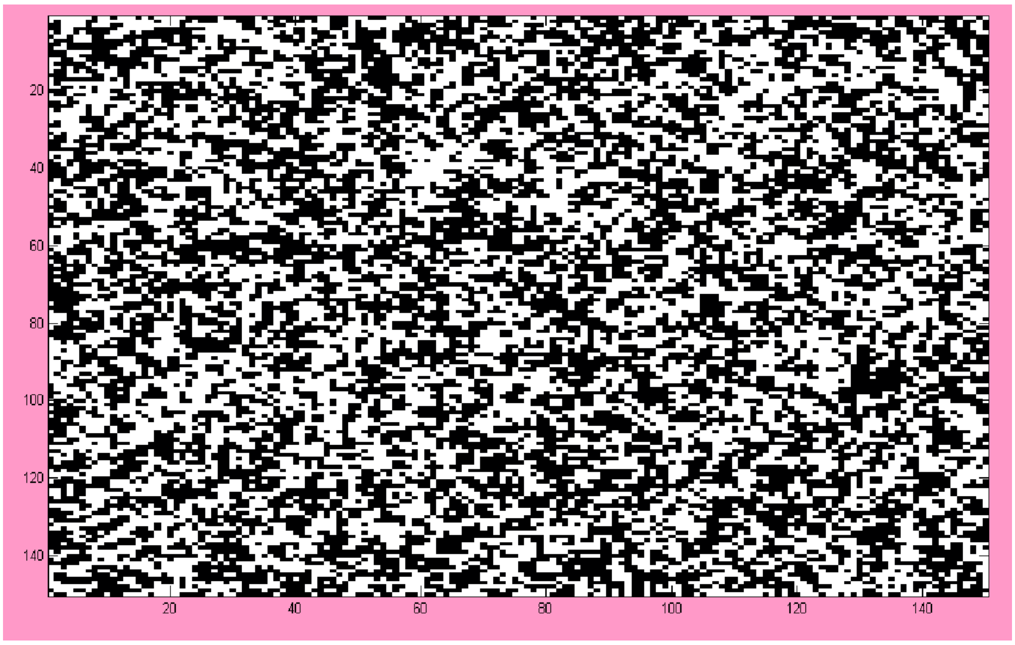

Figure 9: Equilibrium spin configuration at different temperatures around T_c after 15,000 steps for 150x150 square lattices.

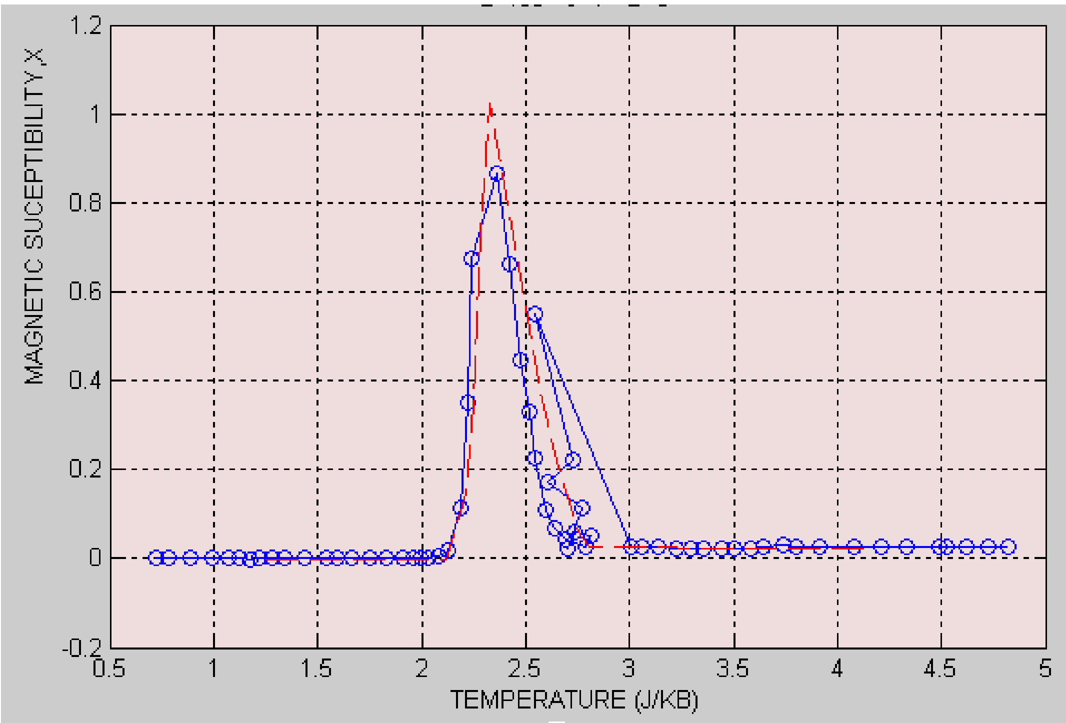

Figure 10: Magnetic susceptibility of a $NiOFe_2O_3$ as a function of temperature for 150x150 square lattices.

CONCLUSION

Phase transitions and critical phenomena are the most universal phenomena in nature. The square-lattice Ising model is the simplest system showing phase transitions and critical phenomena at finite temperatures. The square-lattice Ising model has played a central role in our understanding of phase transitions and critical phenomena. The exact solution of the square lattice Ising model for $NiOFe_2O_3$, a Ferromagnetic with free boundary conditions is not known for systems of arbitrary size. We have obtained the exact solution of the Ising model on the 20 x 20 square lattice and higher square lattice 150x150 with free boundary conditions configuration. We have also discussed the phase transitions and critical phenomena of the square-lattice Ising model using the exact solution on the square lattice with free boundary conditions.

In this work we verify the existence of kink states, and we study their degree of stability. In our simulation, several systems sizes were considered. The study of the static spin correlation between the initial and final configuration shows there that there exist a finite transition temperature Tc, which is independent of the system size. According to our simulation, at T $<T_c$ the kink state is stable, and the degree of stability increases with system size. Our results shows that the critical temperature of $NiOFe_2O_3$ consider is **2.25J/K_B** which is very close to the literature, **2.20J/K_B** [d]

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