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Computational Analysis of *3D* Ising Model Using Metropolis Algorithms

A. F. Sonsin, M. R. Cortes, D. R. Nunes, J. V. Gomes and R. S. Costa

Universidade Federal de Rondônia
Departamento de Física de Ji-Paraná. Rua Rio Amazonas, 351
Jardim dos Migrantes, 78961970 - Ji-Paraná, RO – Brasil

arturfalqueto_sonsin@hotmail.com, mariane_cortess@hotmail.com, danii.nunes@hotmail.com, janygovi@gmail.com and rscosta.unir@gmail.com

Abstract. We simulate the Ising Model with the Monte Carlo method and use the algorithms of Metropolis to update the distribution of spins. We found that, in the specific case of the three-dimensional Ising Model, methods of Metropolis are efficient. Studying the system near the point of phase transition, we observe that the magnetization goes to zero. In our simulations we analyzed the behavior of the magnetization and magnetic susceptibility to verify the phase transition in a paramagnetic to ferromagnetic material. The behavior of the magnetization and of the magnetic susceptibility as a function of the temperature suggest a phase transition around $KT/J \approx 4.5$ and was evidenced the problem of finite size of the lattice to work with large lattice.

1. Introduction

In this work, we used large volume of lattice compared to lattice values used in the literature for Ising model in three dimensions. Therefore we see and evidenced in our calculations the problem of finite size of the lattice.

The Ising Model, even simple, is still of current interest. The model consists of a system of atoms arranged in a regular lattice, described by spin variables that take only two values, +1 and -1. Further, each of these variables interact only with the adjacent former (first neighbors interaction), so that the energy parallel and anti parallel spins is different. Since its creation, the model became the basis for much of the research in the field of critical phenomena and phase transition. The model was proposed by Lenz theme of the doctoral thesis of E. Ising on magnetism, and the first model of the analytical solution has been published by Ising [1].

2. Simulation Computational of the Ising model in 3D

In this work, all simulated physical models are models on the lattice. We understand such models as defined not in the space-time, but the net, an approach the complex n-space-time or simply space. We use the Monte Carlo method [2] to statistical analyzes, and the lattice used were 150^3 200^3 and 250^3. The computational model Ising solution of 3-dimensions can be used to calculate the critical exponent for its corresponding universality class. In 3-dimensions, the Hamiltonian of the model can be written as

$$H = -J \sum_{i,j,k=1}^{N} (S_{i-1,j}S_{i,j} + S_{i,j}\, S_{i+1,j} + S_{i,j-1}\, S_{i,j} + S_{i,j}\, S_{i,j+1} + S_{i-1,k}S_{i,k} + S_{i,k}S_{i+1,k} + S_{i,k-1}S_{i,k} + S_{i,k}S_{i,k+1} + S_{j-1,k}S_{j,k} + S_{j,k}S_{j+1,k} + S_{j,k}S_{j,k-1} + S_{j,k}S_{j,k+1}) - \boldsymbol{H} \sum_{\boldsymbol{i}}^{\boldsymbol{N}} \boldsymbol{s_i}\ . \qquad (1)$$

We do not consider any external force, so $\boldsymbol{H} = 0$. The model Ising studied here is a cube with N spins located at the corners of a cubic lattice. We obtain a magnetization system for different mesh sizes, and temperatures in order to verify the behavior near the phase transition. The magnetization M of a given configuration is simply given by the sum of all the spins in the lattes. And being written by sites (N) as

$$M = \frac{1}{N} \sum_{i}^{N} S_i\ . \qquad (2)$$

The magnetic susceptibility (χ) is the greatness featuring a magnetic material according to their response to an applied magnetic field. The determination of χ can assist in the identification phase transitions. The susceptibility is given by:

$$\chi = \frac{J}{K_B T} (\langle M^2 \rangle - \langle M \rangle^2), \qquad (3)$$

where k_B is the constant Boltzmann, J the exchange term, T the temperature and the magnetization M.

The Cumulant of the Binder is an observational tool for estimating critical points. For different sizes of the lattices , the average magnetization curve always passes through a fixed point, which coincides with the critical point. Thus, generation of magnetization curves for several different sizes of the network can estimate the critical temperature T_c. The place where the curves intersect. Thus, it is a visual characteristic for detection of phase transition, as defined

$$U_4 = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}. \qquad (4)$$

3. Numerical Results

The number of Monte Carlo steps was equal to 10000 and with lattices of the 150^3 , 200^3 and 250^3 to verify the behavior of the magnetization as a function of temperature. And thus estimating a critical temperature of phase transition. Due to the finite size of the lattice problem use the Magnetic Susceptibility and Cumulant of the Binder as a function to estimate an accurate value of the critical temperature.

In Figure 1, we can see that the magnetization behavior is almost the same for different sizes of the lattices: 150^3 , 200^3 and 250^3. Decreasing to reach the critical temperature value and then going to zero after the critical temperature.

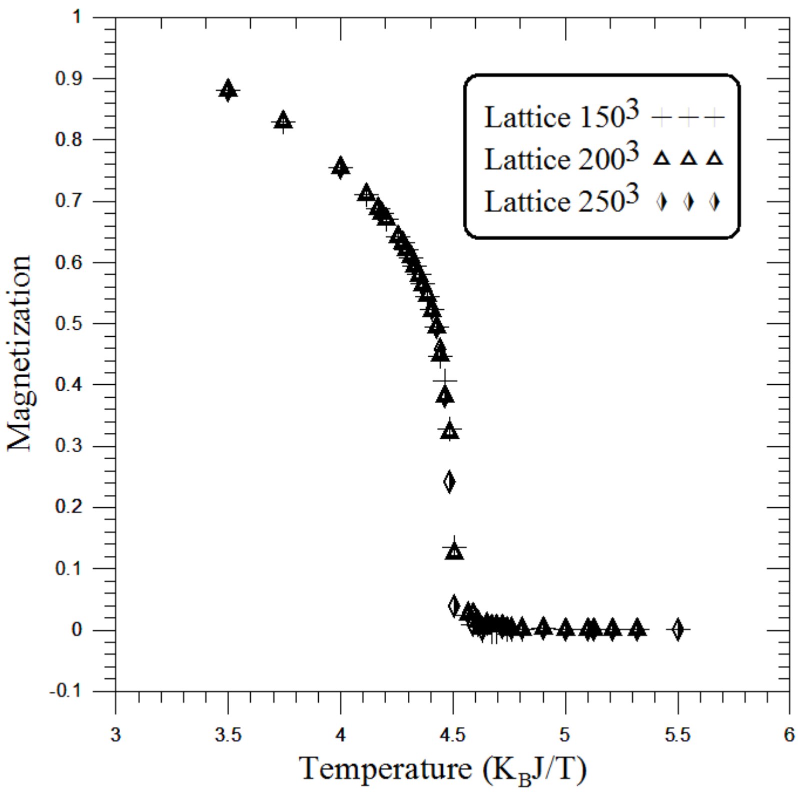

Figure 1: Magnetization as a function of the temperature for lattices of the 150^3, 200^3 and 250^3.

The magnetization is the order parameter of the theory, thus when a sudden change much of its behavior with respect to temperature variation indicates a phase transition of the material. In this case a second-order transition. In this sense we can see in Figure 1 that for temperatures below the critical temperature of the spin is aligned, in other words in the ferromagnetic state. In the region of the critical temperature of the spins begin to clutter indicating a phase transition to the paramagnetic state, that is, where all the spins are disorderly. Just point the critical temperature the magnetization should be close to zero. However, to reach such a situation we should work with infinite lattices $(L^3 \rightarrow \infty)$ which would make them unviable computations. This situation is called the finite size of the lattice, since we can only work with finite limits. Therefore, the magnetization curve with infinite lattices will have an asymptote to reach the critical temperature, indicating a phase transition.

In Figure 2, we can see that with the size of the lattice $L \to \infty$ 1, $U_4 \to 0$ for T > Tc and $U_4 \to 2/3$ for $T < T_c$. Thus, the determination of T_c technique is to make the $U_4 \times T$ chart for different sizes of the lattice (150^3, 200^3 and 250^3). Analyzing the graphic, one can determine the point corresponding to the critical temperature Tc, as the point where all the curves cross. In Figure 2 clearly shows the meeting point of the curves.

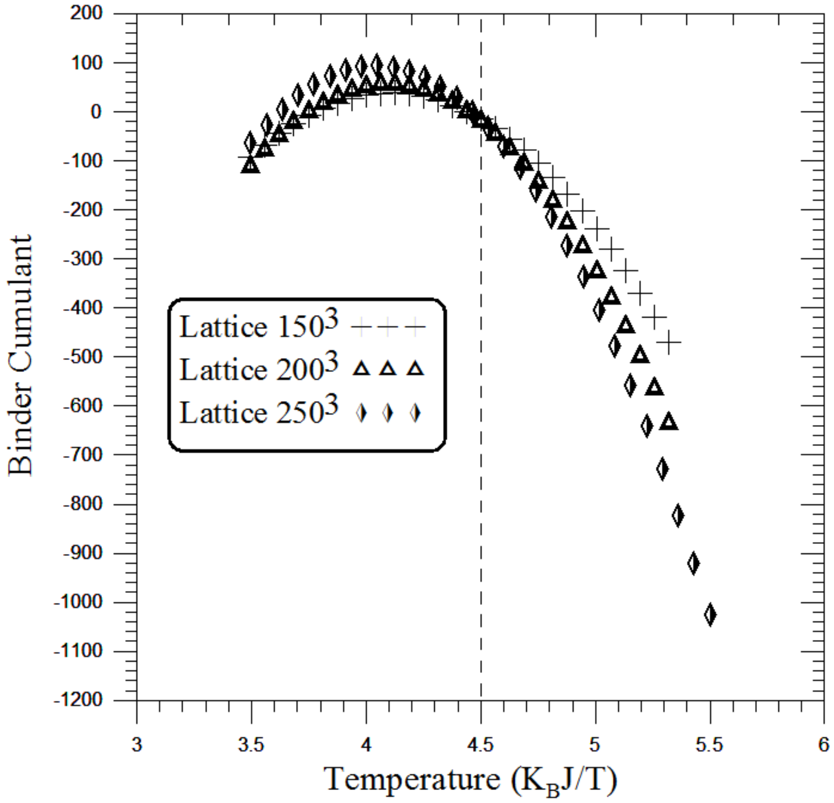

Figure 2:Binder Cumulant as a function of the temperature for lattices of the 150^3, 200^3 and 250^3.

We can see in Figure 3 we get a critical temperature $\boldsymbol{k_B T/J \approx 4.5}$ right next to temperature obtained via computer simulation [3]. To a temperature close to zero, the spins of the lattice tend to align them selves in a similar way to a ferromagnetic even when the **H** field tends to zero. However, after a certain temperature value (called the critical temperature), the spins lose this self-alignment.

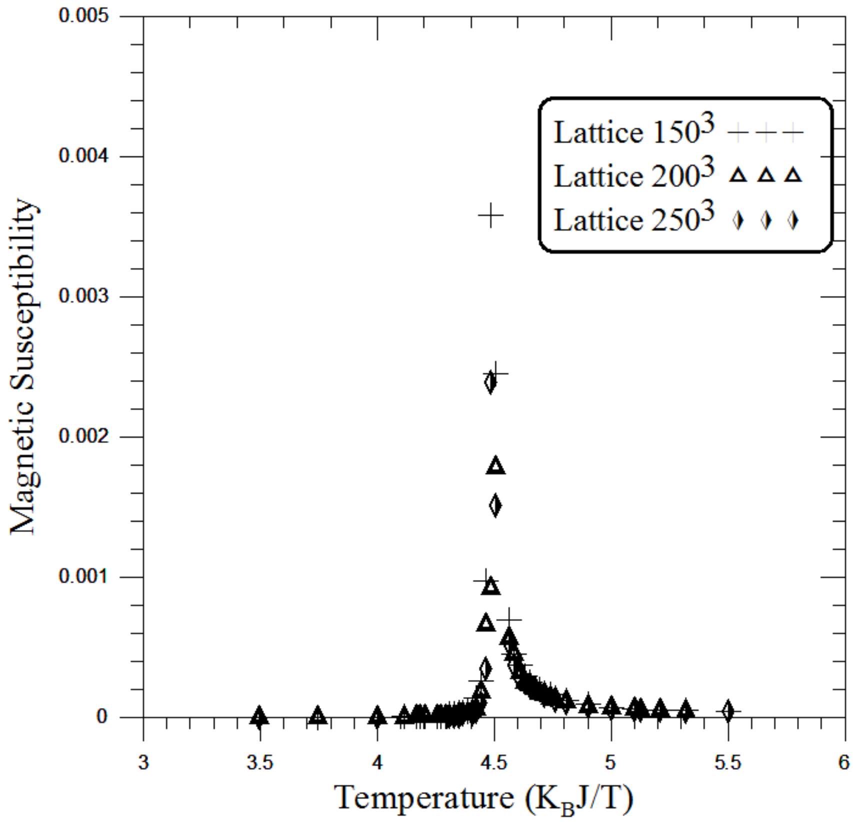

Figure 3: Magnetic Susceptibility as a function of the temperature for lattices of the 150^3, 200^3 and 250^3.

4. Conclusion

We simulate the Ising model with Monte Carlo and we use the Metropolis algorithm to update the distribution of spins. We found that, in the specific case of the three-dimensional Ising model, the Metropolis method is efficient. Studying the system near the phase transition point, we observed that the magnetization goes to zero. The behavior of the magnetization and magnetic susceptibility versus temperature suggest a phase transition around $\boldsymbol{k_B T/J \approx 4.5}$. The value of the critical temperature obtained via computer simulation with large lattice of 150^3, 200^3 and 250^3 was very close to the value found in the literature, via computer simulation for the Ising model in three dimensions with small lattices [3][4][5].

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