3D anisotropic Ising model with Monte Carlo simulation

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Abstract: Magnetization, susceptibility and Curie temperature of 3D anisotropic Ising model for ½ spins system have been investigated by making use of the Monte Carlo simulation. The considered model is parametrized by exchange interaction parameter $J$, anisotropy parameter $\gamma$. The obtained results allowed us to show that for strong coupling case in z axis ($\gamma \gg 1$), the critical temperature is widely to the conventional value of the 3D materials ($T_c = 6.32J$). Thus, an optimal integration of interplanar atoms in z-axis can generate materials that retain the ferromagnetic property even at high temperature.

Keywords: Monte Carlo simulation, Ising model, Anisotropy, phase transition, critical temperature

1. Introduction

The Ising model [1], is a classical model of statistical physics, it provides a simplified microscopic description of ferromagnetic. It has been introduced for the description of magnetism in ferromagnetic materials [2]. But the resolution of this model is not always obvious as a two-dimensional example under nonzero external field conditions and three-dimensional have not yet received an exact analytical solution [3].

There are several approximate theoretical methods that have tried to solve the Ising model such as the average field method [4,6], the series development [7-8], the renormalization group method [9-10] and the finite cluster approximation [10,14]; it has been improved qualitatively and quantitatively the results obtained in the framework of the field method, this is due to the nature of the approximations used, but none of these methods have could give acceptable results. Numerical simulation techniques will therefore be indispensable tools to better understand systems such as the Ising model.

In the present paper we have analyzed the Ising model by a numerical method. The latter facilitates the calculation of the partition function when the model considered is placed on a finite size lattice [15], although this method makes it possible to calculate the values of physical quantities such as; the magnetization, the energy, the specific heat and the susceptibility for a given temperature, note that the accuracy of the results obtained depends on the size considered.

The numerical method with which we worked is the Monte Carlo method [16], this method is used to simulate complex physical phenomena, in several scientific. MC simulation based on the metropolis
method is carried out assuming periodic boundary condition for three-dimensional square lattices of \( L \times L \times L \) with linear lattice size. The difficulty encountered in Monte Carlo simulations with local updates is the critical slowing down near a phase transition. Considerable progress in the development of efficient non-local Monte Carlo algorithms which overcome critical slowing down to a large extent [17-18].

2. Model and formalism

We consider spin \( \frac{1}{2} \) Ising model on a cubic lattice with anisotropic nearest neighbor interactions in Z axis as displayed in Fig.1.

![Fig. 1: Different exchange interaction in 3D anisotropic Ising model.](image)

The Hamiltonian of the system is given by the following expression:

\[
H = -J \sum_{<i,j>} \sigma_i \sigma_j - \gamma J \sum_{<k,l>} \sigma_k \sigma_l - h \sum_i \sigma_i
\]

where \( J \) is the exchange interaction parameter between two nearest-neighbor spins, \( \sum_{<i,j>} \) is summation stand for nearest neighbors spins in OXY plan, \( \sum_{<k,l>} \) is summation stand for nearest neighbors spins in Z axis, \( \gamma \) is the anisotropy parameter and \( h \) is the external longitudinal magnetic field. For \( \gamma = 1 \) case, the considered is equivalent to usual Ising model.

To study the anisotropy effect on some local magnetic properties of the considered system, we use Monte Carlo simulation. This simulation calculation based on Metropolis algorithm, free boundary conditions are applied in the X, Y and Z-directions. Configurations are generated by selecting the sites in sequence through the lattice and making single-spin-flip attempts, which are accepted or rejected according to some probability based on Boltzmann statistics. Starting from different initial conditions, all the Monte Carlo simulations are averaging over different configurations for each starting initial condition. The simulations are carried out for \( N \) spins, where \( N \) is the number of all spin in the lattice.

The aimintation is defined by:

\[
<M> \approx \frac{1}{N} \langle \sum_i \sigma_i \rangle
\]
whereas the susceptibility $\chi$ is given by:

$$\chi = \frac{\partial M}{\partial H} = \frac{(\Delta M)^2}{NK_BT} = \frac{<M^2> - <M>^2}{NK_BT}$$

with $\beta = \frac{1}{K_B T}$, $T$ is the absolute temperature and $K_B$ is the Boltzmann constant taken to be $K_B = 1$ for simplicity.

3. Results and discussion

3.1. Usual Ising model case

The fig. 2 and 3 show the variation of magnetization $M$ as a function of temperature $T$ in weak and strong coupling regime, respectively.

Fig. 2: Magnetization $M$ as a function of temperature $T$ in weak coupling regime at $h=0$

Fig. 3: Magnetization $M$ as a function of temperature $T$ in strong coupling regime at $h=0$
The two figures show that the magnetization decreases as a function of $T$ before being canceled at a critical temperature $T_c$ which represents in this point a phase transition para-magnetic ferromagnetic. The figures show also that this critical temperature increases with $J$. This to precise the $J$ dependency of $T_c$, we note in table 1 the value of $T_c$ for different values of $J$.

| $J$  | $T_c$  | $T_c/J$ |
|------|--------|---------|
| 0.5  | 3.099  | 6.18    |
| 0.7  | 4.389  | 6.27    |
| 1    | 6.690  | 6.69    |
| 2    | 12.90  | 6.45    |
| 3    | 18.60  | 6.2     |
| 4    | 24.20  | 6.05    |

Table 1: Critical temperature for 3D Ising model for different $J$

The obtained results show that the quotient $\frac{T_c}{J}$ is particularly constant, which responds to a number of published results [19-20] which shows that the ratio $\frac{T_c}{J}$ is constant and depends only on the geometry of a spin system. For a one dimensional spin chain, in which no phase transition occurs, Ising initially proposed in his doctoral thesis that there is also no phase transition in higher dimensions which turned out to be a misinterpretation. The Ising model on a two-dimensional without magnetic field was analytically $T_c = 2.269185J$ [21] whereas, at 3D system the critical value is $5.8J$. Thus, we plot in Fig. 4 the variations of $M$ as a function of $T/J$. The curves shows that show the $M$ is independent for $J$ where it vanishes at $\frac{T_c}{J} = 6.30$

![Fig. 4: Magnetization $M$ as a function of $T/J$ at $h=0$](image)

To study the effect of external field $h$ on same local properties of 3D system $\frac{1}{2}$ spins, we plotted in Fig. 5.a and Fig. 5. b the variations of aimantation $M$ as a function of $h$ for $T<T_c$ case and $T>T_c$, respectively. In paramagnetic phase, the curves of Fig. 4.b shows that the aimantation $M$ increases smoothly as a function $h$, especially in the weak coupling regime ($J=0.5$), whit an inflexion point near $(0,0)$. 


Moreover, the curves show that the spins of our consideration of the magnetic field depends on the fact that the effects of interactions between the spins the nearest neighbors favors spin alignment even at low magnetic field. Thus, the magnetization response is larger in the high coupling limit, where the magnetization field is almost independent to $J$. This means that the magnetization response of a ferromagnetic system is independent of the collective effects of spins.

![Fig. 5.a: Magnetization $M$ as a function of external field $h$ in ferromagnetic phase](image)

![Fig. 5.b: Magnetization $M$ as a function of external field $h$ in parramagnetic phase](image)

### 3.2. Anisotropic 3D Ising model case

To show the anisotropy effect on some local properties of 3D spins system, we study the behaviors of aimantation $M$ and the susceptibility $\chi$ as a function of $T/J$ and anisotropy parameter $\gamma$.

First, in Fig. 6 and Fig. 7, we plot the variations of $M$ and $\chi$ for different values of $\gamma$ at $h=0$, respectively.
For weak coupling case in $z$-axis ($\gamma = 0.2$), the corresponding curves show that phase transition occurs at $T_c = 4.1J$. Noting that this critical temperature is particularly very close to one of bidimensional $\frac{1}{2}$ spins system. Thus, in this limit of weak coupling, one can consider that the collective effects between the spin of the $oz$ axis are particularly non-existent. In this cubic lattice can be modelled in non-correlated square lattices.

Whereas, for strong coupling case in $z$ axis ($\gamma = 2$ case), the corresponding curves show that the critical temperature becomes more important where it exceeds widely the conventional value of the three- dimensional materials ($T_c = 6.32J$), thus, an optimal integration of interplanar atoms in $z$-axis can generate materials that retain the ferromagnetic property even at high temperature.
Finally, the Fig. 8 shows \( M \) as a function of \( h/J \) for different values of \( \gamma \) in ferromagnetic phase. The obtained curves show that the aimantation \( M \) varies between -1 and +1 according to an ascending step at a critical value of spins inversion \( h_0 \), where \( |h_0| \) decreases with \( \gamma \).

![Fig.8: Magnetization M as a function of external field for different \( \gamma \).](image)

4. Conclusion

In this paper, we have studied z -anisotropy effect on some local magnetic properties of \( \frac{1}{2} \) spins system described by 3D anisotropic Ising Model. In particular, we have considered \( N \) correlated \( \frac{1}{2} \) spins in 3D cubic lattice with anisotropic nearest neighbor interactions in Z axis. Thus, the ingredients of adapted Ising model are exchange interaction parameter \( J \), anisotropy parameter \( \gamma \) and external magnetic field \( h \). Monte Carlo simulation allowed us to study the behavior of some local properties such as aimantation \( M \) and the susceptibility \( \chi \) as a function of \( J \), \( \gamma \), \( h \) and temperature \( T \).

The obtained results shows that 3D anisotropic Ising model exhibits a phase transition at critical temperature \( T_c \) which is clearly correlated anisotropy parameter \( \gamma \). For weak anistropy (\( \gamma \rightarrow 0 \)), the phase transition occurs at critical temperature which is particularly very close to one of bidimensional \( \frac{1}{2} \) spins system. Whereas, for strong coupling case in z axis (\( \gamma \rightarrow 0 \)) the critical temperature widely the conventional value of the 3D materials (\( T_c = 6.32J \)), thus, an optimal integration of interplanar atoms in z-axis can generate materials that retain the ferromagnetic property even at high temperature.

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