



RESEARCH ARTICLE

MAGNETICS PROPERTIES OBSERVED VIA A CONTOUR FROM XYZ DATA AND Z VALUE AS LABEL FOR EACH XY DATA POINT

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Abstract

The objective of this paper is to describe the ferromagnetic magnetization via a contour from XYZ data and Z value as label for each XY data point. The system has consisted from spin-1/2 atoms with a random exchange interaction J_{ij} . The value of J_{ij} is randomly distributed by a random function. The investigation is based on the effective field theory with correlations. For the appropriate value of the system parameter new descriptions and phenomena of the magnetizations have been obtained. The results show that it is possible to display the ferromagnetic behavior by using the contours with a clear description of the ferromagnetic magnetization. The results are well detailed in the paper.

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Introduction:-

Now a day, almost all the technology [7-14] depends on the magnetic nano-systems [1-6]. The ratio surface/volume is the consequence of several physical properties and phenomenon [15]. Some numerous experimental techniques have been reported to get nanoscales magnetic materials [16-19] and theoretically, the magnetic properties of these nanoparticles have mainly been examined by using the mean-field theory (MFA), the effective-field theory (EFT), and the Monte Carlo simulation (MC) [20-29] with a constant exchange interaction [30,15,22,26]. Otherwise, some investigations have been realized by using a random exchange interaction [31,32,33]. The aim in this paper is to present a way for displaying the ferromagnetic properties (magnetizations) from a contour with XYZ data and Z value as label for each XY data point by using an EFT within the probability distribution technique and a random exchange interaction. On the other hand, as far as we know, the results presented in this paper, have not yet been described in the literature by using a random exchange interaction.

Model and Formalism:-

Consider the nanostructure defined by the following structure.

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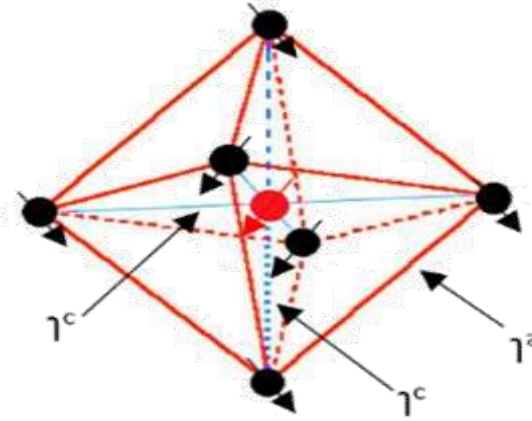


Figure 1:- Nano-octahedral structure.

The red atom is the central spin and the black atoms play the role of the nearest neighbors. In this system, the exchanges interactions (J_s), which linked the atoms on the surface are neglected. Consider only the internal exchange interaction $J_c = J_{ij}$ as a random exchange interaction. Otherwise, the method used for giving the ordered moment is the EFT, well detailed in [34]. Therefore, the transverse Ising model used to investigate the ferromagnetism properties is defined by:

$$H = - \sum_{(ij)} J_{ij} S_{jz} S_{iz} - \Omega \sum_i S_{ix} - h \sum_i S_{iz} \quad (1)$$

where $H = -AS_{iz} + BS_{ix}$

$$A = \sum_{(ij)} J_{ij} S_{jz} + h \text{ and } B = -\Omega.$$

The random exchange interaction is defined by $J_{ij} = \text{rand}(x)$ with $\text{rand}()$ a random function, x the number of exchange interaction possibility, S_{iz} and S_{ix} the components following (Oz) and (Ox) of the spin $S=1/2$, h the magnetic field and Ω the transversal field. Within the formulation of the EFT, accordingly, the different steps for the calculations of the magnetic properties of the system are well detailed in [34,35].

S_{iz} and S_{ix} are represented by the following matrix:

$$S_{iz} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} \text{ and } S_{ix} = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} \quad (2)$$

To calculate the different averages, one has to find the eigenvalues and the associated vectors of the Hamiltonian H [34], which is represented by the following matrix:

$$H = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \quad (3)$$

and the corresponding vectors are given by:

$$E_1 \longrightarrow |\Psi_1\rangle = a_1 \left| \frac{1}{2} \right\rangle + b_1 \left| -\frac{1}{2} \right\rangle \quad (4)$$

$$E_2 \longrightarrow |\Psi_2\rangle = a_2 \left| \frac{1}{2} \right\rangle + b_2 \left| -\frac{1}{2} \right\rangle$$

the quantities $\left| \frac{1}{2} \right\rangle$ and $\left| -\frac{1}{2} \right\rangle$ are the associated vectors of S_z . The coefficients $a_k, b_k (k = 1, 2)$ can be calculated from the following equations[34]:

$$H|\Psi_k\rangle = E_k|\Psi_k\rangle \quad (5)$$

and one has

$$\begin{pmatrix} \frac{A}{2} & \frac{B}{2} \\ \frac{B}{2} & -\frac{A}{2} \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} = \begin{pmatrix} a_k \\ b_k \end{pmatrix} |\Psi_k\rangle \quad (6)$$

Taking account of the conditions of the following normalization of the states:

$$\langle \Psi_k | \Psi_k \rangle = a_k^2 + b_k^2 = 1 \quad (7)$$

Thus, one has:

$$a_k^2 = \frac{B^2}{(A - 2E_k)^2 + B^2} \quad b_k^2 = \frac{(A - 2E_k)^2}{(A - 2E_k)^2 + B^2} \quad (8)$$

From statistics of spin systems, for the operators S_{ir}^α at site i , one has:

$$\langle S_{ir}^\alpha \rangle = \left\langle \frac{\text{Tr}(S_{ir}^\alpha \exp(-\beta H))}{\text{Tr}(\exp(-\beta H))} \right\rangle \quad (9)$$

Where the angular bracket $\langle \dots \rangle$ denotes a canonical thermal average, $\beta = 1/k_B T$, T is the temperature and α is the number of order moment. If the exchange interactions are restricted to nearest-neighbors' interactions only, the evaluation of the inner traces over selected spins in the last equations yields is

$$\langle S_{ir}^\alpha \rangle = \langle F_\alpha(A, B) \rangle \quad (10)$$

Where $\langle F_\alpha(A, B) \rangle = \frac{A}{\sqrt{A^2 + B^2}} \tanh\left(\frac{1}{2} \beta \sqrt{A^2 + B^2}\right)$ if $r=z$: Longitudinal and

$$\langle F_\alpha(A, B) \rangle = \frac{B}{\sqrt{A^2 + B^2}} \tanh\left(\frac{1}{2} \beta \sqrt{A^2 + B^2}\right) \text{ if } r=x: \text{ Transversal}$$

The above thermal averages are valid for a fixed spatial configuration. The step is to carry out the configurational average denoted $\langle \dots \rangle_r$, the quantities are the polarization M^α defined by:

$$M^\alpha = \langle \langle S_{ir}^\alpha \rangle \rangle = \langle \langle F_\alpha(A, B) \rangle \rangle$$

M^α is a function depending of $\sum_{i=0}^N S_{ir}$ like: $F\left(\sum_{i=0}^N S_{ir}\right)$. One introduces the Dirac delta function:

$$\delta\left(y_1 - \sum_{i=0}^N S_{ir}\right) = \int \frac{d\lambda_1}{2\pi} e^{i\left[y_1 - \sum_{i=0}^N S_{ir}\right]} \quad (11)$$

$$\delta\left(y_1 - \sum_{i=0}^N S_{ir}\right) = \int \frac{d\lambda_1}{2\pi} e^{-i\lambda_1 S_{ir}}$$

One has:

$$\left\langle F\left(\sum_{i=0}^N S_{ir}\right) \right\rangle = \int dy_1 \left(y_1 - \sum_{i=0}^N S_{ir}\right) F(y_1) \quad (12)$$

$$F\left(\sum_{i=0}^N S_{ir}\right) = \int dy_1 F(y_1) \int \frac{d\lambda_1}{2\pi} \prod_{i=1}^N e^{-i\lambda_1 S_{ir}}$$

In the approximation of Zernike decoupling of the multiple correlations, one has:

$$\left\langle F\left(\sum_{i=0}^N S_{ir}\right) \right\rangle = \int dy_1 F(y_1) \int \frac{d\lambda_1}{2\pi} \prod_{i=1}^N \langle e^{-i\lambda_1 S_{ir}} \rangle \quad (13)$$

To perform the configurational average on the right-hand side of the last equation, one uses the probability distribution method based on the use of generalized Van der Waander identities [38]. Once done we have:

$$\prod_{i=1}^N \langle e^{-i\lambda_1 S_{ir}} \rangle = \prod_{i=1}^N \left(\sum_{S_{ir}=-1/2}^{1/2} P(S_{ir}) e^{-i\lambda_1 S_{ir}} \right) \quad (14)$$

Where the distribution functions $V(S_{ir})$ are given by:

$$V(S_{ir}) = \frac{1}{2} \left[(1-2p_z) \delta_{S_{ir},-1/2} + (1+2p_z) \delta_{S_{ir},1/2} \right] \quad (15)$$

Taking into account relations above, one gets the following relations for the order moments:

$$M^\alpha = \langle \langle F_\alpha(A, B) \rangle \rangle = 2^{-(N+1)} \sum_{\mu_1=0}^N C_{\mu_1}^N (1+p_z)^{N-\mu_1} \quad (16)$$

$$(1-p_z)^{\mu_1} th(J_\alpha((N-2*\mu_1)+h))$$

In this equation, N represents the coordination number and C_k^n is the binomial coefficients, $C_k^n = \frac{n!}{k!(n-k)!}$ one has

the self-consistent equations for the order moments M^α with the system, which can be solved directly by numerical iteration without any further algebraic manipulations. Then the average total polarization is given by:

$$M = \frac{\sum_{i=1}^n M_i^z}{N} \quad (17)$$

With N the number of spin in the structure.

Results and Discussions:-

The exchange interaction is one among the most important parameter in magnetism. Almost all the articles about magnetism use a constant exchange interaction, by the coupling of the magnetic moments and form magnetically ordered states.

In the presentpaper, a new method bases on the random exchange interaction will be presented. A direct internal random exchange operator "rand()" between moments is introduced in our model. The operatoris closed for having sufficient overlap of the waves functions. The coupling provides a short range and strong coupling, which decrease rapidly and randomly as the ions are separated. Otherwise, when the interatomic distance is small, the electrons spend most of their time in between neighboring atoms. In the case where the atoms are far apart, the electrons spend their time away from each other in order to minimize the electron-electron repulsion.

In the following paper, one considers only the internal exchange interaction (J_C) with a null surface exchange interaction ($J_S=0$). The phase transition from ferromagnetic to paramagnetic depends on the temperature and particularly from the Curie Temperature T_c . Knowing that fact the investigation is based on the description of the ferromagnetic magnetization by using the contour. The contour with XYZ data and Z value as label for each XY data point has been used. Where $X = K_B T/J$: the temperature, $Y = \text{Ran}(J_{ij})$: Random exchange interaction, $Z = M$: Magnetization. The system is described by a spin $S=1/2$, a transverse field $\Omega/J=1.00$, an external field $h/J=0.0$. The aim of the investigation is to display the behaviors of the magnetization according to the temperatures from the Ferromagnetism to Para-magnetism throughout the superparamagnetism as depicted in the figures 1, 2, 3 & 4

For describing the behavior of the magnetization, we've used several exchanges interactions possibilities $x=2, 10, 100, 1000$. We've demonstrated as well that more the random possibility is important more the signature of the magnetization is well displayed as shown the figure 4.

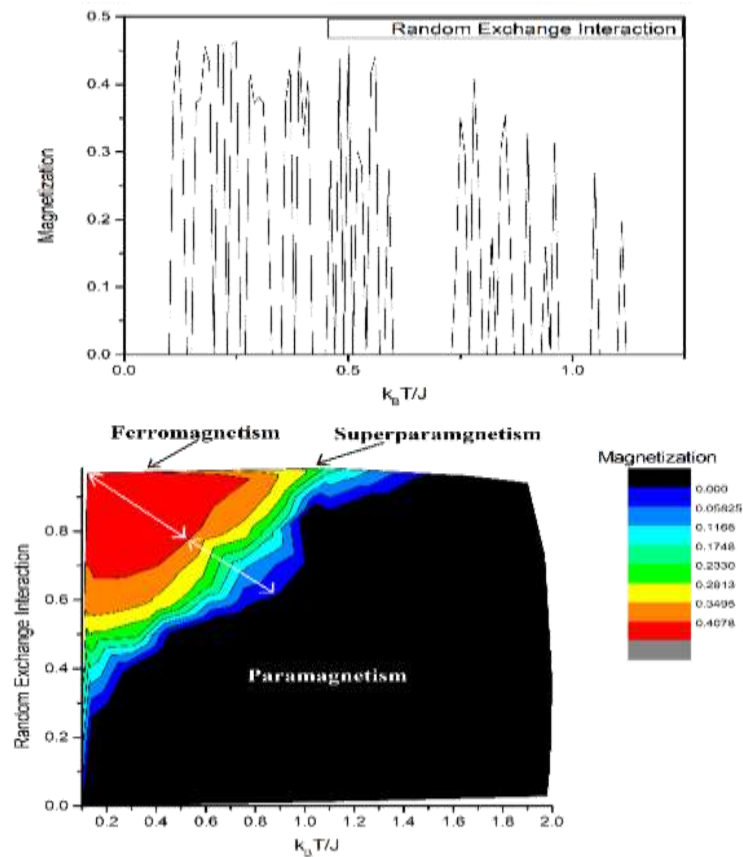


Figure 1:- Thermal variation of the magnetization with a random exchange interaction for $x=2$.

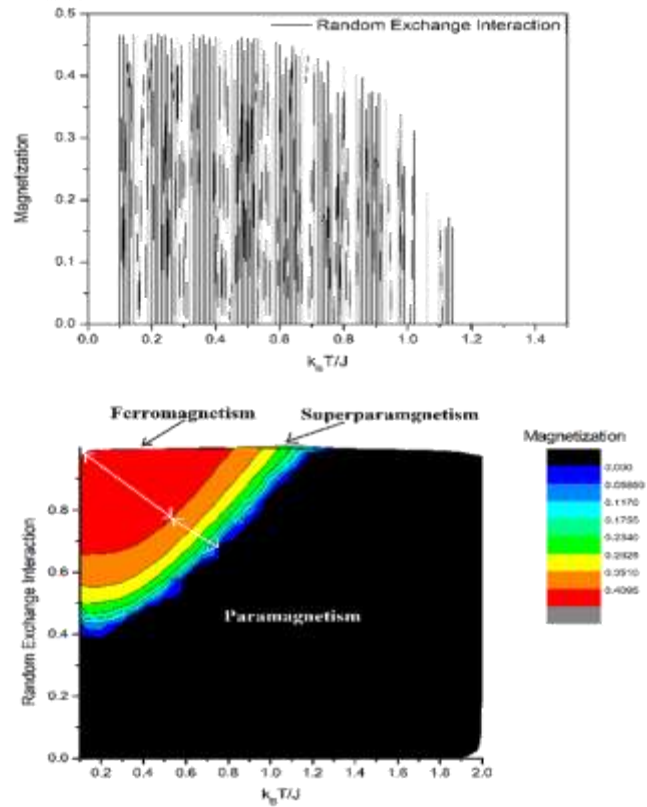


Figure 2:- Thermal variation of the magnetization with a random exchange interaction for $x=10$.

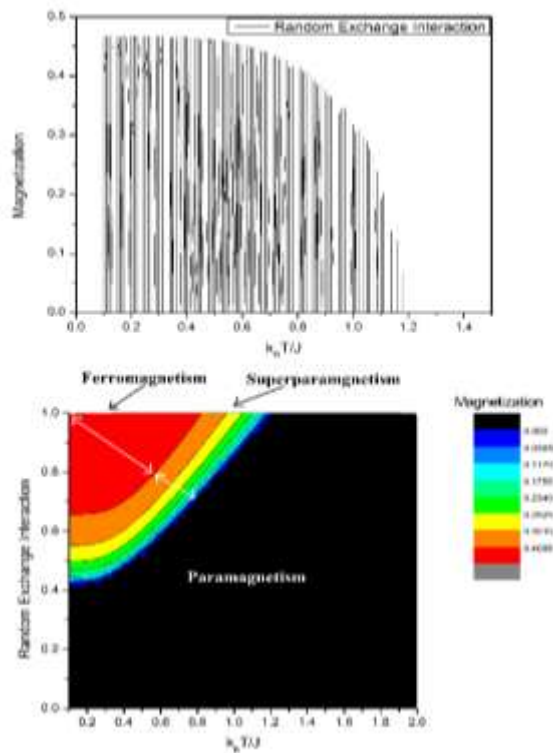


Figure 3:- Thermal variation of the magnetization with a random exchange interaction for $x=100$.

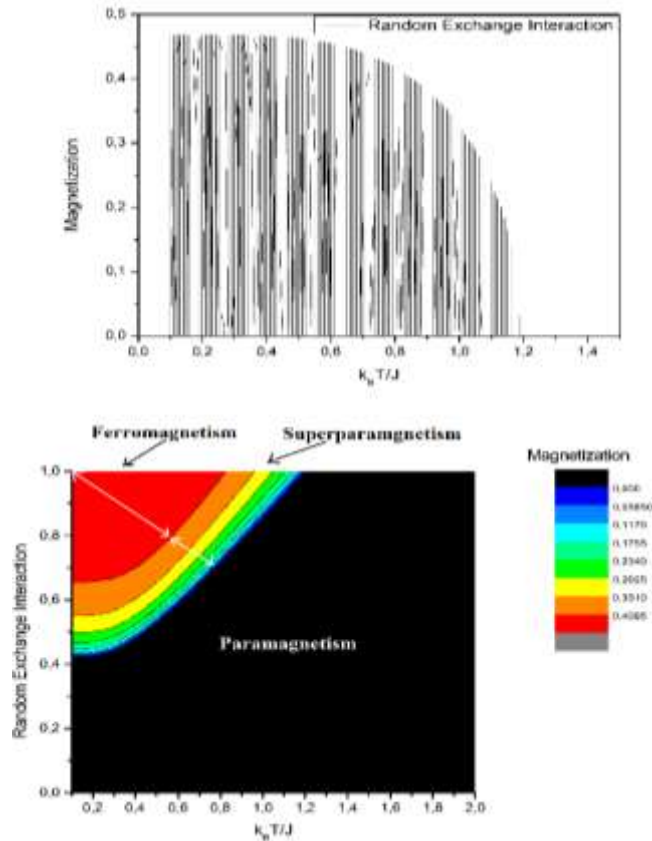


Figure 4:- Thermal variation of the magnetization with a random exchange interaction for $x=1000$.

The ferromagnetic materials are sensitive to the temperatures. Above the Curie temperature (T_C) the materials lose its ferromagnetism properties and become merely paramagnetic.

The random exchange interaction used is the origin of the internal magnetic field, reflects the electrostatic Coulomb repulsion of the electrons on neighboring atoms and the Pauli principle. According to the spin configuration, it exists an average energy between them. That is why the random effects of the exchange interaction and the influence of the temperature, cause a decrease in the spontaneous magnetization at higher temperatures. We've noted as well an important excitation of the spin characterized but a shape change of the magnetizations curves. The fluctuation of the spin from ferromagnetism to paramagnetic is random that is why we observed the spectral magnetization curves displayed in the Figures 1,2,3 & 4.

Otherwise, according to the temperature $k_B T/J$, the transverse field Ω/J and the random exchange interaction J_{re} are used. From the random exchange interaction, the contour with TEM (T =Temperature, E = Exchange interaction and M =Magnetization) data and M value as label for each TE data point has been computed. The results are displayed in figure 1, 2, 3 & 4.

Conclusion:-

In the present paper, we've investigated a nano-structure. With one spin at the center and six spins on the surface connected via a random internal exchange interaction. The surface exchange interaction is neglected. The effects of the random internal exchange interaction have been explained. New ferromagnetic behavior has been observed via a contour with TEM (T =Temperature, E = Exchange interaction and M =Magnetization) data and M value as label for each TE data point. We've shown that with a random exchange interaction another ferromagnetic behavior can be obtained. Otherwise, the investigation of the new phenomena observed with a random internal exchange interaction open a new field in the experimental research of magnetism.

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