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Wetting and layering transitions in a nano-shell structure: Monte Carlo study

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ABSTRACT

The Monte Carlo simulations have been used to study the magnetic properties and the hysteresis of a nano-shell structure composed of four bands, comprising a ferromagnetic spins $\sigma = \pm 1/2$ Ising model. The influence of the surface and inner magnetic fields is responsible for the wetting phenomena and the layering transitions. The behavior of the magnetizations as well as the ground state phase diagrams is presented. We also explore the effect of the external magnetic field, the temperature and the exchange coupling interactions on the hysteresis cycle.

1. Introduction

The study of magnetic properties of a nanostructure is of high interest and it is used for defining the behavior of the nano-particles. Other than that the technological applications developed this domain for achieving profit in different sections, precisely in computer simulations [1,2].

Theoretically, numerous studies have investigated the ferro-magnetic properties of nano-systems, using diverse methods such as mean field (MF) [3], effective field theory (EFT) [4–6] and Monte Carlo simulations (MC) [7–10]. Some studies have found rich critical behavior and many interesting phenomena such as the magnetic and the layering transitions in these systems. By using the Monte Carlo method, a number of characteristic properties may occur in these systems.

On the other hand, Canko et al. [11] investigated the crystal field dependence of the magnetic properties of the mixed two spins Ising nano-cube using the effective field theory (EFT) in which some characteristic phenomena were found such as the tri-critical points. Akıncı et al. have studied the dynamic behavior of a site diluted Ising ferro-magnet under a periodically oscillating magnetic field by means of the effective field theory (EFT) [12,13]. On studying other works by using the Monte Carlo simulation [14], it has been found the dynamic phase transition properties depend on the Hamiltonian parameters such as the magnetic field. Precisely, the corresponding phase diagrams and magnetic properties have been investigated [15,16].

The aim of this paper is to explore the wetting phenomena and layering transitions [17–19] in the spherical geometry showing the rich magnetic properties. Hence, we used the parameters of our Hamiltonian which it showed these phenomena. More precisely, we can examine the effect of coupling in the presence of both inner and surface magnetic fields in our system. On the other hand, we elaborate analytically the corresponding ground state phase diagrams. Indeed, the layering transition temperatures are distinguished in the same system [20]. Then, the magnetic properties are determined using the Monte Carlo method.

In this work, we consecrated our study to demonstrate the influence of the surface and inner magnetic fields, and the coupling on magnetic properties of a ferromagnetic spherical nanostructure, using Monte Carlo simulations. The outline of the paper is organized as follows; in Section 2, we present our model and the formulation of our Hamiltonian. The results and discussions are presented in Section 3, and in Section 4, we present the conclusion.

2. Model and method

In this section, we present the model and the method which will be used in this paper. We consider a ferromagnetic Ising

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model composed of spin σ=½ with two states, in the presence of both the surface and the inner magnetic fields and the external magnetic field. As illustrated in Fig. 1, the system consists of four circular layers. Such structure is similar to that modeled in [21]. The Hamiltonian of this system can be described by the following equation:

$$\mathbf{H} = -J\sum_{i,j}\sigma_i\sigma_j - \sum_i h_i\sigma_i \quad (1)$$

where J represents the coupling exchange interaction between the two first nearest neighbor atoms with spins: $\sigma_i - \sigma_j$. The external longitudinal magnetic field h_i is acting on a site "i" of the shell "k" (k=1, 2, 3, 4) (see Fig. 1). We will study two cases in the following: $H_{s1} = -H_{s2} = -1$ and $H_{s2} = 0$.

A. Case : $H_{s2} = -H_{s1} = -1$

with

$$h_i = \begin{cases} H + H_{s2} & \text{if} : k = 1 \\ H & \text{if} : 1 < k < 4 \\ H + H_{s1} & \text{if} : k = 4 \end{cases} \quad (2)$$

B. Case : $H_{s2} = 0$

with

$$h_i = \begin{cases} H + H_{s1} & \text{if} : k = 4 \\ H & \text{elsewhere} \end{cases} \quad (3)$$

In the above equations, H denotes an external magnetic field, H_{s2} and H_{s1} are the surface magnetic fields applied on layers k=1 and 4, respectively.

The Monte Carlo simulations that we are using are based on the Metropolis algorithm [22]. We perform 10^6 Monte Carlo steps per spin (MCS) and discard the first 10^5 steps to eliminate the initial conditions. The Jackknife method [23] has been used to calculate the error bars. These error bars are not shown in our figures since they take very small values.

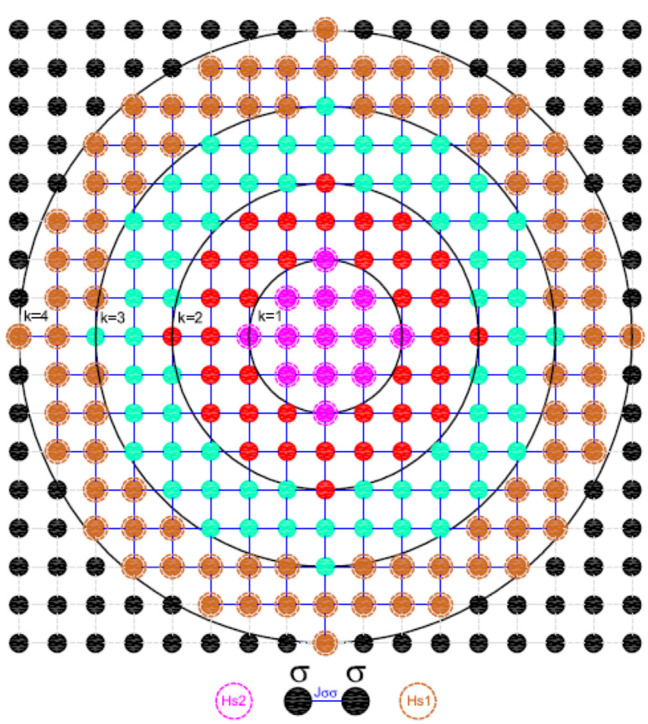

Fig. 1. A sketch of the geometry of the studied system formed by four layers delimited by the rays: R_1, R_2, R_3 and R_4. Each layer contains $N_\sigma^1 = 13$, $N_\sigma^2 = 36$, $N_\sigma^3 = 64$ and $N_s^4 = 84$ spins σ=1/2, respectively.

The total magnetization of each layer, containing N_σ^k spins, can be written as

$$m_\sigma^k = \frac{1}{N_\sigma^k}\sum_{i=1}^{N_\sigma}\sigma_i^k \quad (4)$$

where k=1, 2, 3, 4. The four circles take the radius: $R_1 = 2, R_2 = 4, R_3 = 6$ and $R_4 = 8$ (see Fig. 1). $N_\sigma^1 = 13, N_\sigma^2 = 36, N_\sigma^3 = 64$ and $N_\sigma^4 = 84$ are the number of spins in each shell delimited by the ray circles R_{k-1} and R_k, respectively.

3. Results and discussion

3.1. Ground state phase diagrams

By computing and comparing all possible configuration energies, we can establish the corresponding ground state phase diagrams. Indeed, starting from the Hamiltonian (1) modeling, the study system, and containing the intrinsic and the extrinsic physical parameters. The intrinsic ones are the exchange coupling constant. The extrinsic term is the external magnetic field. When varying such parameters, one can produce many stable topologies corresponding to different energy values. Our algorithm will choose the configurations minimizing the energies produced by the Hamiltonian (1).

Such studied system is represented in Fig. 1, where each layer is formed by band between two circles of rays R_i and R_j. The first layer consists of spins located in circle of ray R_1. The second layer is formed with spins belonging to the surface delimited by the two circles of rays R_1 and R_2 (see Fig. 1). The third layer is located between the two circles of rays R_2 and R_3. The last layer corresponds to the spins situated between the two circles of rays R_3 and R_4.

The ground state phase diagrams, of the studied system, are presented in Figs. 2a–c and 3a–c.The first group of plots corresponds to the case: $H_{s2} = -H_{s1}$, whereas the second one is related to the case H_{s2}=0. These figures are plotted in the planes (J, H), (J, H_{s1}) and (H, H_{s1}) showing different stable configurations. We will use the notations $(\pm1/2, \pm1/2, \pm1/2, \pm1/2)$ to denote that the magnetizations of the layers (k=1, 2, 3 and 4) take the values $\pm1/2$ (see Fig. 1).

Fig. 2a shows that from 2x2x2 × 2=16 possible configurations, only 10 configurations are found to be stable in the plane (J, H). From this figure, we found that the phases $(-1/2, -1/2, -1/2, -1/2)$, $(-1/2, -1/2, +1/2, +1/2)$ $(-1/2, +1/2, +1/2, +1/2)$ and $(+1/2, +1/2, +1/2, +1/2)$ are the only stable ones for positive values of the exchange coupling interaction. The other phases are stable for negative values of this parameter.

In order to show the effect of the surface magnetic field, we plot in Fig. 2b the corresponding stable configuration, for a fixed value of the external magnetic field $H = 1$. Indeed, this figure shows that the only possible configurations are $(+1/2, +1/2, -1/2, -1/2)$, $(+1/2, +1/2, -1/2, +1/2)$, $(+1/2, -1/2, +1/2, -1/2)$, $(-1/2, +1/2, +1/2, -1/2)$, $(+1/2, +1/2, +1/2, -1/2)$, $(-1/2, +1/2, +1/2, +1/2)$ and $(+1/2, +1/2, +1/2, +1/2)$. This figure shows a broken symmetry, due to the fact that we fixed a non-null value the external magnetic field $H = 1$.

The meaning of $J < 0$ is only to underline all the theoretically possible configurations in the ground state phase diagrams. This is shown in Fig. 2a and b. Nevertheless, in this paper we kept the value $J = 1$ for the exchange coupling interaction parameter between different layers.

On the other hand, we plot Fig. 2c, in the plane (H_{s1}, H) for $J = 1$, and found that only six configurations are stable. This figure shows an inverted symmetry regarding the point (H_{s1}=0, $H = 0$), showing the phases $(-1/2, -1/2, +1/2, +1/2)$, $(-1/2, -1/2, -1/2, -1/2)$, $(+1/2, -1/2, -1/2, -1/2)$, $(+1/2, +1/2, -1/2, -1/2)$, $(+1/2, +1/2, +1/2, +1/2)$, and $(-1/2, +1/2, +1/2, +1/2)$.