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Anisotropic Heisenberg model in thin film geometry

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ABSTRACT

The effect of the anisotropy in the exchange interaction on the phase diagrams and magnetization behavior of the Heisenberg thin film has been investigated with effective field formulation in a two spin cluster using the decoupling approximation. Phase diagrams and magnetization behaviors have been obtained for several different cases, by grouping the systems in accordance with, whether the surfaces/interior of the film has anisotropic exchange interaction or not.

1. Introduction

Recently, there has been growing interest both theoretically and experimentally on the finite magnetic materials especially on semi-infinite systems and thin films. The magnetic properties of the materials in the presence of the free surfaces are drastically different from the bulk counterparts. This is because of the fact that, free surface breaks the translational symmetry, i.e. surface atoms are embedded in an environment of lower symmetry than that of the inner atoms [1,2]. If the strength of the surface exchange interaction is greater than a critical value, the surface region can exhibit an ordered phase even if the bulk is paramagnetic and it has a transition temperature higher than the bulk one. This fact has been observed experimentally [3–5].

The development of the molecular beam epitaxy technique and its application to the growth of thin metallic films has stimulated renewed interest in thin film magnetism. In a thin film geometry, one important question is dependence of the thermodynamic properties and Curie temperature of the film on the thickness of the film. It was experimentally found that, the Curie temperature and the average magnetic moment per atom increase with the increasing thickness of the film [6,7]. This thickness dependent Curie temperature also has been measured in Co [8], Fe [9] and Ni [10] films.

In order to get insight on the phase transition characteristics and thermodynamic properties of thin films, it is valuable in theoretical manner to solve related models in thin film geometry such as Hesinberg and Ising models. One class of the films which exhibit a strong uniaxial anisotropy [11] can be modeled by Ising model. These systems have been widely studied in literature by means of several theoretical methods such as Monte Carlo (MC) simulations [12], mean field approximation (MFA) [13] and effective field theory (EFT) [14]. In the Ising case, the study of ferroelectric films treated by transverse Ising model (TIM) is more common in the literature, since fabricated ferroelectric thin films such as Barium titanate $BaTiO_3$ and Strontium titanate $SrTiO_3$ [15–17] have a lot of technological applications in optoelectronics [18] and microelectronics [19]. The TIM on the thin film geometry can be solved by a variety of techniques such as MFA [20] and EFT [21]. Besides, within the EFT formulation, the effect of the dilution on the phase diagrams and magnetic properties of the ferroelectric thin films (by means of the TIM) has been studied [22] and also long range interactions have been taken into account [23]. In order to simulate more realistic models, different exchange interactions have been defined and different transverse fields have been considered on the surface and bulk, which anticipates the mimics of the surface effects within the framework of EFT [24]. Another improvement of the Ising thin film models is the consideration of amorphisation of the surface due to environmental effects, and these realizations have also been solved using EFT [25]. There are also higher spin Ising thin films, e.g. spin-1 Ising thin films have been studied [26,27].

Although the Ising model has been studied on the thin film geometry widely, less attention was paid on the Heisenberg model on thin film geometry, in comparison with the Ising model. Thin films which do not exhibit a strong uniaxial anisotropy require to solve the Heisenberg model in the thin film geometry. In order to see the effect of the presence of the surface in the system on the critical and thermodynamical properties, Heisenberg model on a semi infinite geometry has been solved using a wide variety of techniques such as Green function method [28], renormalization group technique [29], MFA [30], EFT [31–33], high temperature series expansion [34,35]. Besides, critical and thermodynamic properties of the bilayer [36,37] and multilayer [38] systems have been investigated within the cluster variational method in the pair approximation. As in the case of Ising counterpart, Heisenberg model in a thin film geometry has been solved in a limited case. For instance, Heisenberg model on a thin film geometry with Green function method [39–41], renormalization group technique [42], MFA [30], EFT [43,44] and MC [45,46], are among them.

The aim of this work is to determine the effect of the anisotropy in the exchange interaction on the phase diagrams and magnetization

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behavior of the Heisenberg thin film. For this aim, the paper is organized as follows: In Section 2 we briefly present the model and formulation. The results and discussions are presented in Section 3, and finally Section 4 contains our conclusions.

2. Model and formulation

The schematic representation of the thin film can be seen in Fig. 1. System is infinitely long in x and y direction, while finite in z direction. Thin film can be treated as a layered structure which consists of interacting L parallel layers. Each layer (in xy plane) is defined as a regular lattice with coordination number z. When we choose $z = 4$, this means that each layer has square lattices and each nearest neighbor layer has interaction. The Hamiltonian of the thin film is given by

$$\mathcal{H} = -\sum_{<i,j>}\left(J_{ij}^x s_i^x s_j^x + J_{ij}^y s_i^y s_j^y + J_{ij}^z s_i^z s_j^z\right) - \sum_i H_i s_i^z \quad (1)$$

Where s_i^x, s_i^y and s_i^z denote the Pauli spin operators at a site i. J_{ij}^x, J_{ij}^y and J_{ij}^z stand for the anisotropy in the exchange interactions between the nearest neighbor spins located at sites i and j and H_i is the longitudinal magnetic field at a site i. The first sum is carried over the nearest neighbors of the lattice, while the second one is over all the lattice sites. The exchange interaction components $(J_{ij}^x, J_{ij}^y, J_{ij}^z)$ between the spins on the sites i and j take the values according to the positions of the nearest neighbor spins. The two surfaces of the film have the intralayer coupling components (J_1^x, J_1^y, J_1^z). The interlayer coupling between the surface and its adjacent layer (i.e. layers 1,2 and L–1,L) is denoted by (J_2^x, J_2^y, J_2^z). For the rest of the layers, the interlayer and the intralayer couplings are assumed as (J_2^x, J_2^y, J_2^z).

We use the two spin cluster approximation as an EFT formulation, namely EFT-2 formulation [47], which was first proposed in Ref. [48] for Ising systems. EFT can provide results that are superior to those obtained within the MFA, due to the consideration of self spin correlations, which are omitted in the MFA. Nevertheless, EFT cannot handle fluctuations correctly. In EFT-2 approximation, we choose two spins (namely s_1 and s_2) in each layer and treat interactions exactly in this two spin cluster. In order to avoid some mathematical difficulties, we replace the perimeter spins of the two spin cluster by Ising spins (axial approximation) [49]. After all, by using the differential operator technique and decoupling approximation (DA) [50], we can get an expression for the magnetization per spin, i.e. $m = \left\langle \frac{1}{2}\left(s_1^z + s_2^z\right)\right\rangle$. In the thin film geometry number of L different representative magnetizations for the system by following the procedure given in Ref. [44] can be given as,

$$\begin{aligned} m_1 &= \left\langle \Theta_{1,1}^3 \Theta_{2,2}\right\rangle f_1(x,y,H_1,H_2)|_{x=0,y=0} \\ m_k &= \left\langle \Theta_{2,k-1}\Theta_{2,k}^3\Theta_{2,k+1}\right\rangle f_2(x,y,H_1,H_2)|_{x=0,y=0}, k = 2,3,\ldots,L-1 \\ m_L &= \left\langle \Theta_{2,L-1}\Theta_{1,L}^3\right\rangle f_1(x,y,H_1,H_2)|_{x=0,y=0}. \end{aligned} \quad (2)$$

Here m_i, $(i = 1,2,\ldots,L)$ denotes the magnetization of the i^{th} layer. The operators in Eq. (2) are defined via

$$\Theta_{k,l} = [A_{kx} + m_l B_{kx}]\left[A_{ky} + m_l B_{ky}\right] \quad (3)$$

where

$$\begin{aligned} A_{km} &= cosh\left(J_k^z \nabla_m\right) \\ B_{km} &= sinh\left(J_k^z \nabla_m\right), \quad k = 1,2; m = x,y. \end{aligned} \quad (4)$$

The functions in Eq. (2) are given by

$$f_n(x,y,H_1,H_2) = \frac{x+y+H_1+H_2}{X_0^{(n)}} \frac{sinh\left(\beta X_0^{(n)}\right)}{cosh\left(\beta X_0^{(n)}\right) + exp(-2\beta J_n^z) cosh\left(\beta Y_0^{(n)}\right)} \quad (5)$$

where

$$\begin{aligned} X_0^{(n)} &= \left[\left(J_n^x - J_n^y\right)^2 + (x+y+H_1+H_2)^2\right]^{1/2} \\ Y_0^{(n)} &= \left[\left(J_n^x + J_n^y\right)^2 + (x-y+H_1-H_2)^2\right]^{1/2} \end{aligned} \quad (6)$$

with the values $n = 1,2$. In Eq. (5), we set $\beta = 1/(k_B T)$ where k_B is Boltzmann constant and T is the temperature.

Magnetization expressions given in closed form in Eq. (2) can be constructed via acting differential operators on related functions. The effect of the exponential differential operator to an arbitrary function $F(x)$ is given by

$$exp(a\nabla)F(x) = F(x+a) \quad (7)$$

with any constant a.

With the help of the binomial expansion, Eq. (2) can be written in the form

$$\begin{aligned} m_1 &= \sum_{p=0}^{3}\sum_{q=0}^{3}\sum_{r=0}^{1}\sum_{s=0}^{1} K_1(p,q,r,s) m_1^{p+q} m_2^{r+s} \\ m_k &= \sum_{p=0}^{1}\sum_{q=0}^{1}\sum_{r=0}^{3}\sum_{s=0}^{3}\sum_{t=0}^{1}\sum_{v=0}^{1} K_2(p,q,r,s,t,v) m_{k-1}^{p+q} m_k^{r+s} m_{k+1}^{t+v} \\ m_L &= \sum_{p=0}^{3}\sum_{q=0}^{3}\sum_{r=0}^{1}\sum_{s=0}^{1} K_1(p,q,r,s) m_L^{p+q} m_{L-1}^{r+s} \end{aligned} \quad (8)$$

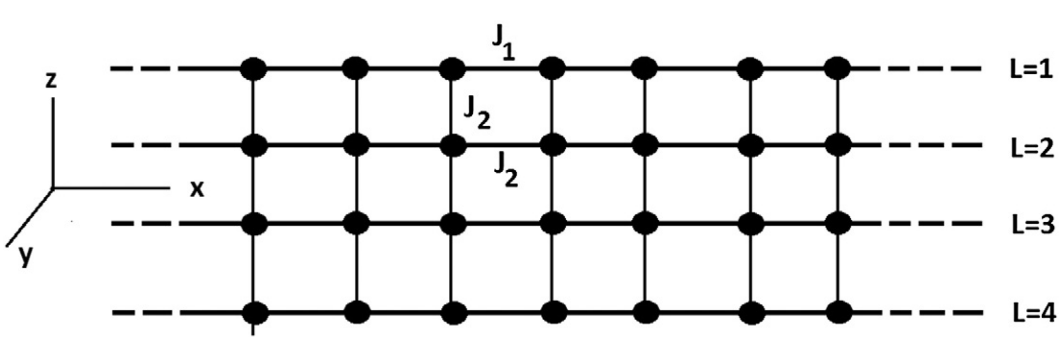

Fig. 1. Schematic representation of the thin film.