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# Magnetic properties of a nanoscaled ferrimagnetic thin film: Monte Carlo and effective field treatments

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ABSTRACT

The magnetic properties of a spin-1/2 Ising nanoscaled thin film with anti-ferromagnetic interfacial coupling between the surface and the next layer are investigated. This has been done by using the two theoretical frameworks of the effective field theory, based on a probability distribution method, and the Monte Carlo simulation. The influence of the system parameters on the phase diagram, on the internal energy and on some other magnetic proprieties of the system are examined. We have found that the nanoscaled thin film exhibits a compensation temperature and triple hysteresis loops for appropriate values of the system parameters.



## 1. Introduction

Over the last years, the magnetic nanoparticle systems have attracted much attention, both for their fundamental interest as well as for possible technological applications [1,2], such as information storage devices, magnetic recording media and biomedical [3–5]. From the theoretical point of view, many characteristic phenomena in magnetism of the nanoparticle have been investigated [6–11]. Using the Monte Carlo simulation (MCS), Feraoun et al. [12] have examined the magnetic properties of a ferromagnetic nanowire on a hexagonal lattice. They have observed that the compensation temperature can appear for appropriate values of the system parameters. Kaneyoshi has investigated the phase diagram [13] and the magnetization [14] of a transverse Ising nanowire by using the effective field theory (EFT) with correlation. He has found that magnetic properties are strongly influenced by the surface and the finite size. On the other hand, Akıncı has studied the effects of the anisotropy in the exchange interaction on the critical behavior of a Heisenberg thin film [15], and the influence of the random magnetic field distributed with the Gaussian distribution centered at zero on the phase diagrams of a transverse Ising thin film [16]. Keskin et al. [17] have investigated the hysteresis behaviors of the Ising nanowire system, and have found that the phase transition temperature and the hysteresis behavior of the system are in good agreement with both theoretical and experimental results.

Moreover, MCS has been used to examine the thickness dependence of the hysteresis properties in Ising thin films [18]; the hysteresis behaviors of maghemite nanoparticles have been studied by the MCS [19]. Dynamics and scaling of low-frequency hysteresis loops in nanomagnets are investigated by solving numerically the Landau-Lifshitz-Gilbert equation [20]. By the use of the EFT with correlation the hysteresis behaviors and the longitudinal susceptibility are investigated [21,17]. Recently we have examined in Ref. [22] the magnetic properties and hysteresis loops of a Blume-capel nanowire in a crystal field by using

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the MCS, the hysteresis behavior of nanotubes, composed of a ferromagnetic core with spin-1 atoms, surrounded by a ferromagnetic shell with spin-1 atoms with ferro- or anti-ferromagnetic interfacial coupling, has been also studied in Ref. [23].

The ferromagnetic thin film has been extensively discussed, due to a broad range of applications, especially in recording applications [24]. Oxide thin films with perovskite-type structure (such as Barium titanate $BaTiO_3$ and Strontium titanate SrTiO3) have been fabricated [25–27], and novel physical properties have been found in ferroelectric thin films which have many application areas in technology [28], such as optoelectronics [29], microelectronics [30] and random access memory [31]. The ferromagnetic thin films [32], and the ferromagnetic/antiferromagnetic ($Ni/Fe_xMn_{1-x}$) bilayer [33] have been studied experimentally and theoretically. Wang et al. [34] have examined the magnetic properties and critical behavior of a molecular-based magnetic film $AFe^{II}Fe^{III}(CeO_4)_3$. A number of characteristic phenomena, such as the possibility of two and three compensation points, are found. In recent work, Jiang et al. [35] have investigated the magnetic and the thermodynamic properties of a nanoscale multilayer ferrimagnetic films. They have shown that two compensation points exist in a range of surface physical parameters. In a series of works on ultra-thin spin-1/2 and spin-1 Ising (or transverse Ising) films with bond and site dilutions at the surfaces [36–42], Kaneyoshi has investigated the phase diagrams and magnetizations by the use of the effective-field theory with correlations. Some unconventional phenomena have been found in the magnetic properties of these systems, such as the appearance of abroad maximum in the variation of transition temperature ($T_c$) as a function of r ($r = J_1/J$) for the site dilution, while such a phenomenon has not been obtained for the bond dilution. In Ref. [43], the phase diagrams of an ultra-thin spin-1 Ising film with a negative single-ion anisotropy have been investigated, in order to clarify how the tricritical behavior can be obtained in such ultra-thin film with dilutions. In a previous work [44], the MCS and the EFT have been used to study the effects of the surface parameters and the random longitudinal field, on the critical and compensation behaviors of a spin-1/2 Ising nanowire.

Taking into account all the above studies, it has been noticed that, the phase diagrams and the hysteresis behavior of the Ising nanoscaled thin films with spin-1/2 atoms have not been investigated. Therefore, this paper aims at examining the influence of the temperature, of the exchange interaction coupling in the surface, and of the interfacial coupling between the surface and the bulk on the magnetic and the hysteresis behaviors of the Ising nanoscaled thin film with spin-1/2, within the framework of the effective field theory based on a probability distribution method (EFT) and the Monte carlo simulation (MCS). We have examined the effects of the interaction coupling constant and the temperature on the phase diagram, on the internal energy and on some other magnetic proprieties of the system.

The outline of this paper is as follows. In section 2, we present the model and the formalism. In section 3, the results and the discussions are given, followed by a brief conclusion.

## 2. Formalism

We consider an Ising nanoscaled thin film of $L_z = 5$ layers on a simple cubic lattice with free surface parallel to the (001) plan. The hamiltonian of the system is given by

$$\mathscr{H} = -\sum_{\langle i,j\rangle} J_{ij}\sigma_i^z\sigma_j^z - H\sum_{\langle i\rangle}\sigma_i^z \tag{1}$$

Where $\sigma_i^z$ is the component of the spin ±1/2 at site i; $J_{ij}$ is the strength of the exchange interaction between the spins at nearest-neighbor sites i and j, and H is the longitudinal magnetic field.

We assume $J_{ij} = J_s$ if both spins belong to surface layers, $J_{ij} = J_1$ between the surface and the bulk, and $J_{ij} = J$ otherwise. The surface exchange interaction $J_s$ is often defined as

$$J_s = J(1 + \Delta_s) \tag{2}$$

### 2.1. Effective field theory (EFT)

Using the (EFT) with the probability distribution, which is based on a simple site cluster comprising just a simple selected spin labeled i and the neighboring spins, with which it directly interacts. The total hamiltonian is split into two parts, $\mathscr{H} = \mathscr{H}_i + \mathscr{H}'$, the part $\mathscr{H}_i$ includes all those terms in the hamiltonian containing the spin i. In this case "classical system" $\mathscr{H}_i$ commute with $\mathscr{H}'$, the starting point of a single cluster theory is a set of a formal identities of the type:

$$\langle\sigma_i^z\rangle = \langle\frac{Tr_{(i)}\sigma_i^z\exp(-\beta\mathscr{H}_i)}{Tr_{(i)}\exp(-\beta\mathscr{H}_i)}\rangle = F_m(y_n) \tag{3}$$

$\beta = \frac{1}{K_B T}$, with $K_B$ is the Boltzmann constant and T the absolute temperature, <....> indicates usual canonical ensemble average for a given configuration and sums run over all possible configurations of atoms environing or lying on the site, respectively.

Using the EFT with a probability distribution technique the longitudinal magnetization is given by: