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Thermal and magnetic properties of ternary mixed Ising nanoparticles with core–shell structure: Effective-field theory approach

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ABSTRACT

We propose a ternary Ising spins (1/2, 1, 3/2) model to investigate the thermal and magnetic properties of magnetic nanoparticles with core–shell structure within the framework of the effective-field theory with correlations. The center site of the core is occupied by $\sigma = \pm 1/2$ spin, while those surrounding the center site are occupied by $S = \pm 1$, 0 spins and the shell sites are occupied by $m = \pm 1/2, \pm 3/2$ spins. Thermal behaviors of the core and shell magnetizations, susceptibilities and internal energies as well as total magnetization are examined. In order to confirm the stability of the solutions we also investigate the free energy of the system. According to the values of Hamiltonian parameters, the system undergoes first- and second-order phase transitions. Phase diagrams are calculated and discussed in detail. We find that the system exhibits a tricritical point, reentrant and five different type (Q, P, R, S and W) of compensation behaviors that strongly depend on interaction parameters. The results are in good agreement with some experimental and theoretical results.

1. Introduction

Molecular-based magnetic materials, which are of interest because they are insulating, transparent, and offer the opportunity of creating novel lattice architecture [1,2], have been studied by using the ternary mixed Ising system for the last 15 years. Among these compounds, a particular interest has been paid to Prussian blue analogs that offer advantages over the other magnets, such as photoinduced magnetism [3–5], anisotropic photoinduced magnetism in thin films [6,7], a charge-transfer-induced spin transitions [8–12], and hydrogen storage capacity [13]. Moreover, these materials may exhibit at most two compensation points [14,15]. The ternary alloy AB_pC_{1-p} composed of Prussian blue analogs has been extensively studied by well-known methods in equilibrium statistical physics. For example, the magnetic properties of a mixed ferro-ferrimagnetic ternary alloy of the type AB_pC_{1-p} consist of three different metal ions with ternary Ising spins (1/2, 1, 3/2) using the effective-field theory (EFT) with correlations [16,17] and the mean-field approximation (MFA) [18] and exact recursion relations (ERR) on the Bethe lattice [19,20]; with Ising spins (1, 3/2, 5/2) within the MFA [21–24], EFT [25], the Monte Carlo (MC) simulations [26] and the ERR on the Bethe lattice [27]; with spins (3/2, 2, 5/2) by employing the MFA [28–30], with Ising spins (1/2, 1, 5/2) by using the MC simulations [31], and with Ising spins (1/2, 3/2, 5/2) within the framework of the ERR on the Bethe lattice [32,33] have been investigated. Moreover, many more experimental works have been done about Prussian blue analogs (see[34–45] and references therein).

On the other hand, in the past two decades, magnetic nanoparticles are a subject of great interest for both experimental and theoretical researchers, due to their technological and biomedical applications such as sensors, molecular imaging devices, high density magnetic recorders. [46–49] and biomedical applications such as magnetic resonance imaging, drug delivery, cell and tissue targeting or hyperthermia [50–54]. Moreover, their magnetic properties are quite different from those of the bulk and are greatly affected by the particle size [55–58]. Magnetic properties of nanoparticles have been studied within various Ising systems consisting of core–shell structures by using a variety of theoretical techniques. An early attempt to study the magnetic behavior of nanoparticles was made by Wang et al. [59]. They used a spin-1/2 system to investigate phase transitions in magnetic alloy nanoparticles by the variational cumulant expansion. Iglesias and Labarta [60,61] studied finite-size and surface effects in maghemite nanoparticles [60] as well as role of surface disorder on magnetic properties and hysteresis of a single maghemite ferromagnetic (FM) nanoparticle [61] by employing the spin-1/2 Ising system within Monte Carlo (MC) simulations. Crisan et al. [62] investigated the magnetic properties of core–shell-type nanoparticles with non-magnetic core and the FM shell within MC simulation by using the spin-1/2 Ising system.

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Leite and Figueiredo [63] have considered a simple spin-1/2 Ising model for an antiferromagnetic (AFM) small particle, which was simulated on a two-dimensional hexagonal structure, with the AFM core interactions and a disordered magnetic surface by mean-field calculations and MC simulations.

Kaneyhoshi [64–66] studied phase diagrams [64], magnetizations [65] and the possibility of a compensation point [66] of nanoparticles with a core–shell structure by using the effective-field theory (EFT) with correlations. Yalçın et al. [67] investigated the magnetic properties of noninteracting monodomain nanoparticles based on the pair approximation. Kaneyoshi and Yalçın et al. were also used the spin-1/2 Ising system. Zaim et al. [68] used the binary mixed spins (1/2, 1) Ising system to study the effects of the shell coupling and the AFM interface coupling on the behavior of the hysteresis loops and the compensation temperature of an Ising ferrimagnetic core/shell nanocube by the use of MC simulations. In the study, the sites of core occupied by spins withtake the spin values $\pm 1/2$, while those of the shell site are occupied by spin values ± 1, 0. Zaim and Kerouad [69] studied the magnetic properties and the critical behaviors of a single spherical nanoparticle, consisting of a FM spin-1/2 core surrounded by FM spins-1 or -3/2 with the AFM interface coupling, by using MC simulations. The phase diagrams and the magnetic properties of a random field spin-1 Ising nanotube with FM exchange interfacial coupling by using an effective field theory based on a probability distribution method are examined by Magoussi et al. [70]. Zaim et al. [71] investigated the magnetic behavior of mixed spins (1, 3/2) spherical nanoparticle on a simple cubic lattice by MC simulation technique. Yüksel et al. [72] applied Monte Carlo simulations based on standard Metropolis algorithm to investigate the phase diagrams of a FM cubic nanoparticle (nanocube) with a spin-3/2 core surrounded by a spin-1 shell layer with AFM interface coupling. Recently, Jiang et al. [73] studied the magnetic properties of a nanoparticle described by the transverse Ising model with single-ion anisotropic, which consists of a concentric spin-3/2 core and a hexagonal ring spin-5/2 shell coupled with a FM interlayer coupling, which are studied by the effective-field theory with self-spin correlations. Kantar et al. [74] investigated the magnetic properties of two-dimensional (2D) nanoparticles, which consist of a FM spin-1/2 core surrounded by FM spin -3/2 with the FM and AFM interface couplings, within the framework of the EFT with correlations. Finally, we should also mention that FM and AFM nanoparticles have been also studied within the Green function [75–78] and the concept of the magnetometric tensor field [79].

In spite of these studies, to the best of our knowledge, magnetic properties of nanoparticles are not studied by the model of ternary mixed Ising system. Therefore, in this paper we propose a ternary Ising spins (1/2, 1, 3/2) model to investigate the thermal and magnetic properties of magnetic nanoparticles with core–shell structure within the framework of the effective-field theory with correlations. In particular, thermal behaviors of the core and shell magnetizations, susceptibilities and internal energies as well as the total magnetization are studied. We also investigate the free energy of the system to confirm the stability of the solutions. Phase diagrams are calculated and discussed in detail. We also investigate the compensation behaviors which are of crucial importance in the area of thermomagnetic recording devices.

The outline of this paper is as follows. In Section 2, we give the model and formalism upon which the EFT with correlation is based. In Section 3, we present the numerical results and discussions, followed by a brief summary.

2. Model and formulation

The schematic representation of ternary mixed Ising nanoparticles with core–shell structure is displayed in Fig. 1. The center

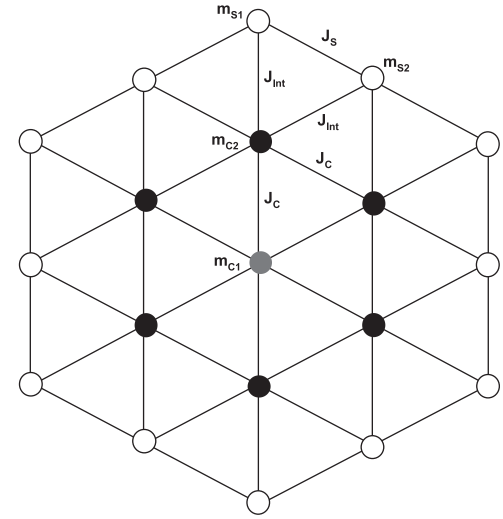

Fig. 1. Schematic representation of a ternary mixed Ising nanoparticles.

site of the core, marked with filled circles, is occupied by $\sigma = \pm 1/2$ spin, while those surrounding the center site are occupied by $S = \pm 1$, 0 spins and the shell sites, marked with open circles, are occupied by $m = \pm 1/2, \pm 3/2$ spins. Each spin is connected to the nearest-neighbor spins with an exchange interaction. Therefore, the magnetic nanoparticles are modeled by ternary Ising spins (1/2, 1, 3/2) system with the following interaction Hamiltonian:

$$H = -J_S \sum_{\langle ij \rangle} m_i m_j - J_C \left(\sum_{\langle mn \rangle} S_m S_n + \sum_{\langle pr \rangle} S_p \sigma_r \right) - J_{Int} \sum_{\langle kl \rangle} S_k m_l - D \left(\sum_i m_i^2 + \sum_k S_k^2 \right) - h \left(\sum_i m_i + \sum_k S_k + \sum_r \sigma_r \right), \tag{1}$$

where J_S and J_C are the exchange interaction parameters between the two nearest-neighbor magnetic particles at the surface shell and core, respectively, and J_{Int} is the interaction parameter between the two nearest-neighbor magnetic particles at the surface shell and the core shell. D is the crystal field. The indexes $\langle ij \rangle$, $\langle mn \rangle$ and $\langle pr \rangle$, and $\langle kl \rangle$ denote the summations over all pairs of neighboring spins at the shell surface, core and between shell and core, respectively. The surface exchange interaction is often defined as $J_S = J_C(1+\Delta_S)$ in order to clarify the effects of surface exchange interaction on the physical properties in the nanosystem [80–85].

Now, we use the EFT with correlations to obtain the EFT equations for the model. This method was first introduced by Kaneyoshi and co-workers [86,87], which is a more advanced method dealing with Ising systems than the mean-field approximation (MFA), because it considers the correlations. Within the framework of the EFT with correlations, one can easily find the magnetizations m_{S1} and m_{S2}, the quadrupole moments q_{S_1} and q_{S2}, the octupolar moments r_{S_1} and r_{S2} on the surface shell, and the magnetizations, namely m_{C1} and m_{C2}, the quadrupole moment q_{C2} on the core, as coupled equations, for the mixed Ising nanoparticles system as follows:

$$m_{S1} = [A(a) + B(a) m_{S2} + C(a) q_{S2} + D(a) r_{S2}]^2 \left[q_{C2} \left(\cosh(J_{Int} \nabla) - 1 \right) + m_{C2} \sinh(J_{Int} \nabla) + 1 \right] f_1(x)|_{x=0}, \tag{2a}$$

$$m_{S2} = [A(a) + B(a) m_{S1} + C(a) q_{S1} + D(a) r_{S1}]^2 [q_{C2} (\cosh(J_{Int} \nabla) - 1) + m_{C2} \sinh(J_{Int} \nabla) + 1]^2 f_1(x)|_{x=0}, \tag{2b}$$