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RESEARCH ARTICLE

Ferrimagnetism in the Mean-field Approximation of a Mixed Spin Ising Nanowire System

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Abstract

A ferrimagnetic mixed spin square Blume-Capel Ising nanowire system consists of spin-1 core and spin-3/2 outer shell has been investigated. The general formula for the temperature dependence of the equilibrium magnetization of the system is presented. The ferrimagnetic core-shell nanosystem shows a compensation point when the exchange interactions are changed at various values of the single-ion anisotropies of shell sublattices and core ones, respectively. So, one can examine interesting phenomena are compensation behaviors and the free energy of the nanosystem, where these phenomena found that the mixed-spin square Blume-Capel Ising nanosystem which is being considered has two spin compensation temperatures in the range of $-0.8 \leq D_B|J_1| \leq -0.4$, when $J_3 = -0.7$, for two different values of core anisotropy for sublattices of atoms A, $D_A|J_1| = 0$, and $D_A|J_1| = 1.0$, respectively.

Introduction

Recently, much attention has directed towards the understanding of magnetization processes and related applications. Thus, magnetic nanowires have provided a highly successful test ground for understanding the microscopic mechanisms that determine macroscopically important parameters in the different applications [1, 2]. The development of ferromagnetic nanowire arrays has revealed various unusual properties relevant to applications in high density data storage devices and in bioengineering applications [3]. B. Deviren and Y. Sener studied the magnetic properties of a mixed spin Ising nanoparticles with core/shell structure by using the effective-field theory with correlations.

The authors found that the system gives new behaviors under the effects of crystal field, core and shell interactions and interface coupling on the phase diagrams. In this research we have investigated the magnetic properties of a ferrimagnetic mixed spin-1 and spin-3/2 square Blume-Capel Ising nanowire system, for a series of molecular based magnets, which is numerically solved by using the mean-field approximation (MFA), in order to clarify the physical background for the characteristic phenomena observed in the ferrimagnetic mixed nanowire models. The work is outlined as follows. In Section 2, we introduce briefly the basic framework of the mean-field theory and give the Hamiltonian of a ferrimagnetic mixed spin-(1, 3/2) square Blume-Capel Ising nanowire system. In Section 3, the numerical results for the phase diagrams, the magnetization of the system are studied in detail. Finally, conclusion is presented in Section 4.

Model and Formalism

The proposed model consists of a ferrimagnetic square nanowire consists of the spin-1 core for atoms A and spin-3/2 outer shell for atoms B, respectively, as shown in Fig.1.

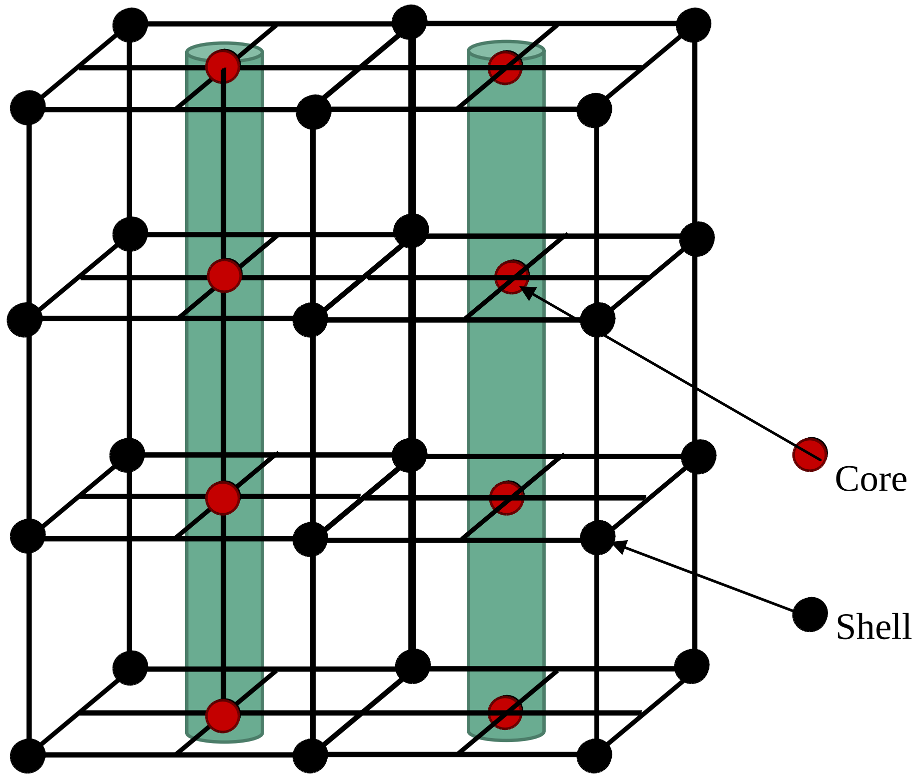

Fig.1: Square Blume-Capel Ising nanowire with core-shell structure. Each square represents a plaquette consisting of one core spin and four shell spins

The Hamiltonian of the nanosystem, in the absence of external magnetic field, is written as [4],

$$H=-J_1\sum S_i^A S_j^B - J_2\sum S_i^A S_i^A - J_3\sum S_j^B S_j^B - D_A\sum S_i^{A^2} - D_B\sum S_j^{B^2} \quad (1)$$

Where $\left(S_i^A, S_j^B\right)$ takes the values $\left(\pm 1, \pm\frac{3}{2}\right)$; and D_A is a magnetic anisotropy acting on A-atoms (core anisotropy), D_B is a magnetic anisotropy acting on B-atoms (shell anisotropy). J_1 Is the nearest neighbour exchange parameter between magnetic atoms across the core and the outer shell. J_2 Is the nearest neighbour exchange parameter between magnetic atoms in the core. J_3 Is the exchange interaction at the outer shell. The free energy of the nanosystem is obtained from a mean field calculation of the Hamiltonian based on the Bogoliubov inequality [5]:

$$A \le \Phi = A_0 + \langle H - H_0 \rangle_0 \quad (2)$$

Where A is the Gibbs free energy of H given by relation (1), that:

$$A = -k_B T \ln Z \quad (3)$$

A_0 is the Gibbs free energy of a paramagnetic phase and H_0 a trial Hamiltonian depending on variational parameters, that:

$$A_0 = -k_B T \ln Z_0 \quad (4)$$

Z, Z_0 are the true partition function and trial one respectively. In this research we consider one of the possible choices of H_0, namely:

$$H_o = -\sum_i [\lambda_1 s_i^A + \gamma_A (s_i^A)^2] - \sum_j [\lambda_2 s_j^B + \gamma_B (s_j^B)^2] \quad (5)$$

S_i^A Taking the values of spins for core-atoms, and S_j^B taking the values of spins for shell-atoms. Whereas λ_1, λ_2, γ_A, and γ_B are the variation parameters related to the different spins and the anisotropies of the two sublattices proposed(i.e., the core and shell anisotropies), respectively. Then, the approximated free energy can be obtained by minimizing the right side of equation (2) with respect to variational parameters mentioned above. Thus, Eq. (2) can be expressed as,

$$f \equiv \frac{\Phi}{N} = -\frac{1}{\beta}\{\ln(a+1) + 4\ln b\} + J_1 z_1 m_A m_B + J_2 z_2 m_A^2 + 4J_3 z_3 m_B^2 \qquad (6)$$

With,

$$a = 2e^{\beta D_A}\cosh\beta\lambda_1 \ ; \ \lambda_1 = J_1 z m_B + 2J_2 z m_A \ ; \ z_1 = z_2 = z_3 = z$$

And,

$$b = 2e^{\frac{9}{4}\beta D_B}\cosh\frac{3}{2}\beta\lambda_2 + 2e^{\frac{1}{4}\beta D_B}\cosh\frac{1}{2}\beta\lambda_2 \ ; \ \lambda_2 = \frac{1}{4}J_1 z m_A + 2J_3 z m_B$$

With,

$$m_A = \frac{2\sinh\{t_1 z_1 m_B + t_2 z_2 m_A\}}{2\cosh\{t_1 z_1 m_B + t_2 z_2 m_A\} + 2e^{-\beta D_A}} \qquad (7)$$

$$m_B = \frac{1}{2}\,\frac{3\sinh\{\frac{3}{2}t_1 z_1 m_A + \frac{3}{2}t_3 z_3 m_B\} + e^{-2\beta D_B}\sinh\{\frac{1}{2}t_1 z_1 m_A + \frac{1}{2}t_3 z_3 m_B\}}{\cosh\{\frac{3}{2}t_1 z_1 m_A + \frac{3}{2}t_3 z_3 m_B\} + e^{-2\beta D_B}\cosh\{\frac{1}{2}t_1 z_1 m_A + \frac{1}{2}t_3 z_3 m_B\}} \qquad (8)$$

Where, $\beta = \frac{1}{K_B T}$, z is the coordination number of the lattice.

It is worth noting that the ferrimagnetic case shows that the signs of sublattice magnetizations are different, and there may be a compensation point at which the total longitudinal magnetization per site is equal to zero [6].

Results and Discussion

The magnetic phase transitions have been investigated numerically by the use of mean-field approximation (MFA), in order to clarify the physical background for the characteristic phenomena observed in the ferrimagnetic mixed nanowire models. The effect of single-ion anisotropies (i.e., crystal fields) on the compensation phenomenon has been taken into consideration. Besides, we have shown the effect of exchange interactions on the magnetization curves and the phase transitions of these systems. Let us consider the thermal variation dependence of the total magnetization for a mixed spin-1 and spin-3/2 square Blume-Capel Ising nanowire as shown in Fig.2, Fig.3, respectively.

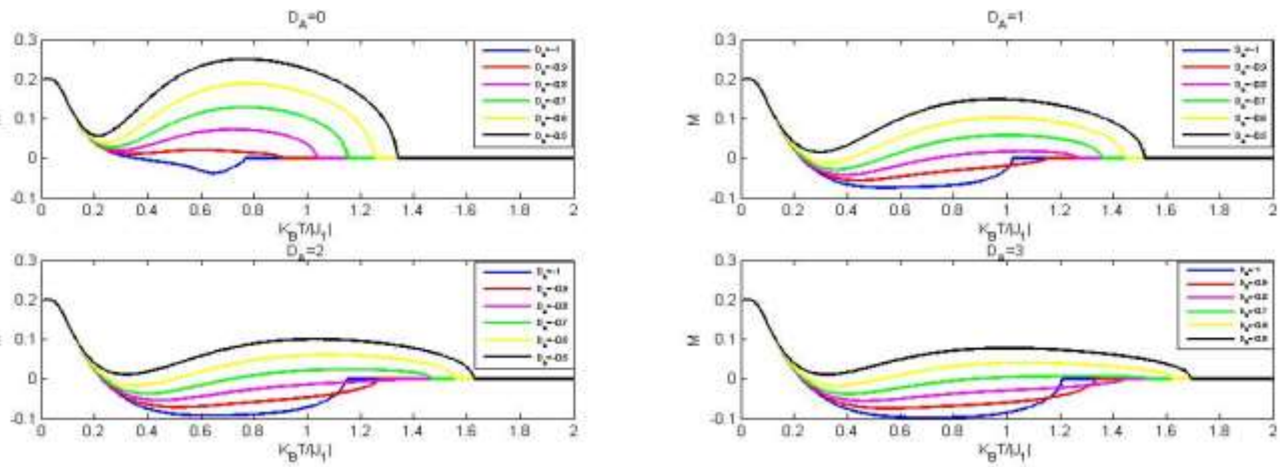

Fig.2: the temperature dependences of the total magnetization M for a ferrimagnetic mixed-spin square Ising nanowire with, J_1=-1, J_2= - 1, J_3= - 0.75

We found some compensation behaviors for square-type nanowire, at different values of $D_A|J_1|$ and $D_B|J_1|$, when $J_1=-1, J_2=-1, J_3=-0.75$, respectively. Fig.2. Reveals interesting phenomena regards compensation temperatures in the range of $0 \le D_A|J_1| \le 3$, for different values of $D_B/|J_1| = -1.0,-0.9,-0.8,-0.7,-0.6,-0.5$. One can observe, Fig.2, when $1 \le D_A|J_1| \le 3$, shows a multicompensation behavior for different $D_B/|J_1| = -1.0,-0.9,-0.8,-0.7,-0.6,-0.5$, respectively. It is worth to note that the compensation points are induced by the presence of magnetic anisotropy for the atom-B, which is possible only in the ferromagnetic phase. These sublattice magnetizations undergo a cancellation but it is still incomplete so there is a residual spontaneous magnetization in the system (M≠0), this is evidence to the antiferromagnetic nearest neighbor interactions [7]. This interaction tends to align neighboring spins in opposite directions as the system's temperature is increased, so the direction of this residual magnetization can switch due to the thermal agitation. The compensation behaviors shown in Figs.(2,3) indicate the crossing points between the magnitudes of m_A and m_B which prove the eligibility of Eqs.(7) and (8). B.

Boughazi et al studied a hexagonal nanowire consisting of a ferromagnetic spin-1/2 core and spin-3/2 outer shell coupled with ferrimagnetic interlayer coupling by the use of Monte Carlo simulation. The authors have plotted the total magnetization versus the temperature for some selected values of $R_S(J_S/J)(0, 0.05, and\, 0.10)$, respectively. As is seen from these parameters that the system exhibits one compensation temperature. One can compare our interesting results with those ones [8].

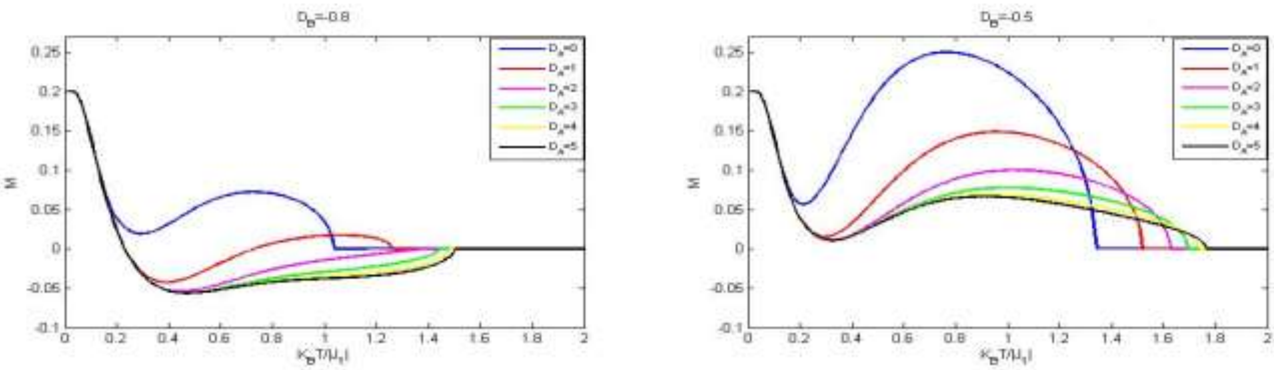

Fig.3: The temperature dependences of the total magnetization M for a ferrimagnetic mixed-spin square Ising nanowire at different values of D_A and D_B, when J_1=-1, J_2= - 1, J_3= - 0.75

On the other hand, Fig.3 shows the temperature dependences of the total magnetization M for a ferrimagnetic mixed spin Ising nanowire system, with $J_1=-1, J_2=-1, J_3=-0.75$. One has observed that nanosystem has two compensation points when $D_A|J_1| = 1.0$, and $D_B|J_1| = -0.8$, for $J_1=-1, J_2=-1, J_3=-0.75$. This is in a good agreement with the possibility of two compensation points in other nanosystems which have been discussed as in Refs. [9, 10].

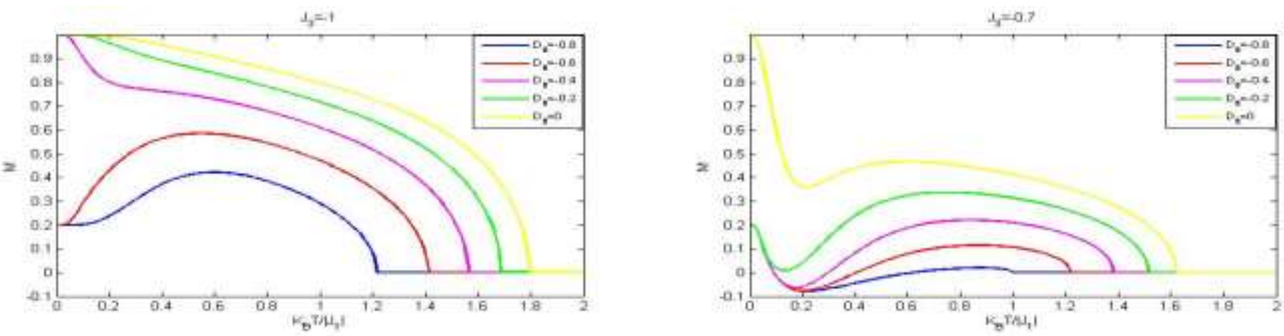

Fig.4: The temperature dependences of the total magnetization M at constant values of D_A=0 and different values of D_B for J_1= J_2= - 1

Now let us examine the temperature dependences of the total magnetization M for the mixed spin Ising nanowire ferrimagnetic system with, J_1=-1, J_2= - 1, for J_3= - 1.0, and J_3= - 0.7, respectively. One can see Fig.4, that the system has two compensation points at a fixed value of $D_A|J_1| = 0$ and different values of $D_B|J|$, in particular for J_3= - 0.7. This is in a good agreement with the possibility of two compensation points in another nanosystem which has been discussed as in Ref. [10].

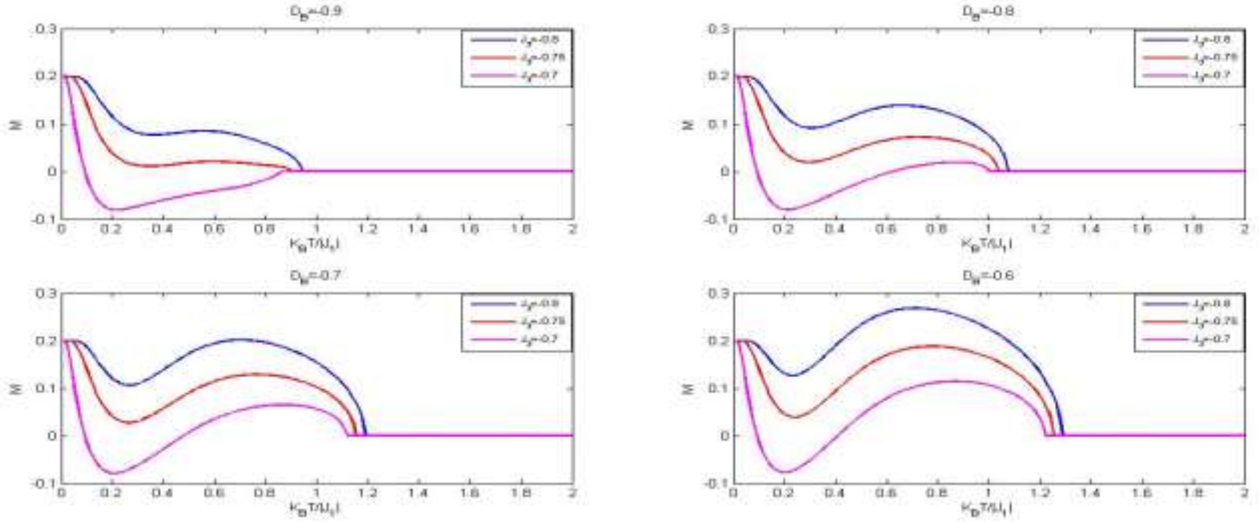

Fig.5: the temperature dependences of the total magnetization m at constant values of D_A=0 and different values of D_B, when J_2= - 1, for J_3= - 0.8,-0.75,-0.7, respectively

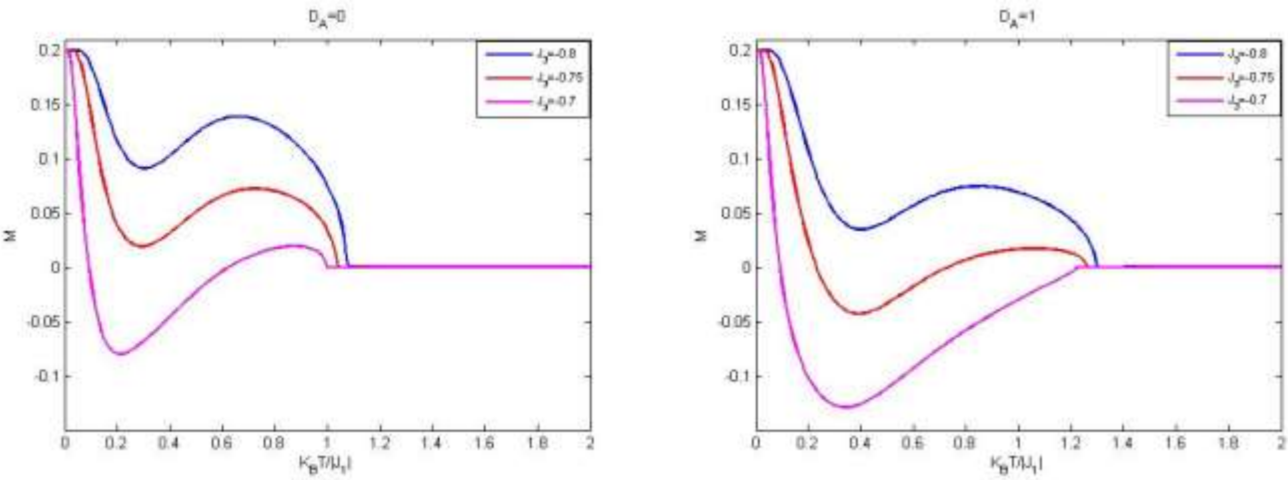

Fig.6: The thermal dependence of the total magnetization m at constant values of D_B = - 0.8 and different values of D_A, when J_2= - 1, for J_3= - 0.8,-0.75,-0.7, respectively

From the two Figures (5, 6), one has found interesting features, i.e., the possibility of multicompensation temperatures are particularly induced, when $D_A|J_1| = 0$, $J_3 = -0.7$, in the range of $-0.8 \le D_B|J_1| \le -0.6$, respectively.

Conclusions

We have investigated a ferrimagnetic mixed spin-(1, 3/2) square Blume-Capel Ising nanowire system by using the mean-field treatment. The effect of single-ion anisotropies (i.e., crystal fields) on the compensation phenomenon has been taken into consideration. The magnetic anisotropies have carefully been changed so that one can examine interesting phenomena are compensation behaviors where these phenomena found that the mixed-spin square Blume-Capel Ising nanosystem which is being considered has one compensation temperature when the core anisotropy is in the range $1.0 \le D_A/|J_1| \le 5.0$ at $D_B/|J_1| = -0.8$, for J_1=-1, J_2=-1, J_3=-0.75. Besides, our nanosystem has two spin compensation temperatures in the range of $-0.8 \le D_B|J_1| \le -0.4$, when $J_3 = -0.7$, for two different values of core anisotropy for sublattices of atoms A, $D_A|J_1| = 0$, and

$D_A|J_1| = 1.0$, respectively. It has been shown that the appearance of spin compensation points is independent of D_A; however D_A influences the magnitudes of these points in the temperature space. On the other hand, from the experimental point of view, it has been synthesized quasi-one-dimensional heterotrinuclear complex $[NiCr_2(bipy)_2(C_2O_4)_4(H_2O)]H_2O$, which shows a rare case of anti-ferromagnetism between $Ni(II)S = 1$ and $Cr(III)S = 3/2$

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