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Mean-Field Solution of a Mixed Spin-3/2 and Spin-2 Ising Ferrimagnetic System with Different Single-Ion Anisotropies

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ABSTRACT

The mixed spin-3/2 and spin-2 Ising ferrimagnetic system with different single-ion anisotropies in the absence of an external magnetic field is studied within the mean-field theory based on Bogoliubov inequality for the Gibbs free energy. Second-order critical lines are obtained in the temperature-anisotropy plane. Tricritical line separating second-order and first-order lines is found. Finally, the existence and dependence of a compensation points on single-ion anisotropies is also investigated for the system. As a result, this mixed-spin model exhibits one, two or three compensation temperature depending on the values of the anisotropies.

Keywords: Ising Model; Magnetization; Compensation Point; Critical Lines; Tricritical Point; Anisotropy; Mixed-Spin

1. Introduction

During the past several decades, both experimental and theoretical studies have accumulated in the area of molecular-based magnetic materials [1-3]. These materials include bimetallic molecular-based magnetic materials in which two kinds of magnetic atoms alternate regularly and exhibit ferrimagnetic properties and therefore they are well interpreted by the use of mixed-spin Ising systems which have less translational symmetry than their single-spin counterparts since they consist of two interpenetrating unequivalent sublattices. For this reason, in recent years, there have been many theoretical studies of the mixed-spin systems.

One of the earliest and simplest of these models to be studied was the mixed spin Ising system consisting of spin-1/2 and spin-S (S > 1/2) in a uniaxial crystal field. The model for different values of S (S > 1/2) has been investigated by acting on honeycomb lattice [4-6], as well as on Bethe lattice [7,8], mean field approximation [9], effective field theory with correlations [10-14], cluster variational theory [8], renormalization-group technique [15] and Monte-Carlo simulation [16-18]. The mixed-spin Ising systems consisting of higher spins are not without interest. Indeed, the magnetic properties of mixed spin-1 and spin-3/2 Ising ferromagnetic system with different single-ion anisotropies have been investigated with the use of an effective field theory [19,20], mean field theory [21], a cluster variational method [22] and Monte Carlo simulation [23].

Recently, the investigations have been extended to high order mixed spin ferrimagnetic systems (mixed spin-3/2 and spin-2 ferrimagnetic system and mixed spin-3/2 and spin-5/2) in order to construct their phase diagrams in the temperature-anisotropy plane and to consider magnetic properties of these systems.

Bobak and Dely investigated the effect of single-ion anisotropy on the phase diagram of the mixed spin-3/2 and spin-2 Ising system by the use of a mean-field theory based on the Bogoliubov inequality for the free energy [24].

Albayrac also studied the mixed spin-3/2 and spin-2 Ising system with two different crystal-field interactions on Bethe lattice by using the exact recursion equations [25]. Bayram Deviren *et al.* have used the effective field theory to study the magnetic properties of the ferrimagnetic mixed spin-3/2 and spin-2 Ising model with crystal field in a longitudinal magnetic field on a honeycomb and a square lattice [26].

In this paper, we therefore apply the mean-field theory based on Bogoliubov inequality for the Gibbs free energy to study the effects of two different single-ion anisotropies in the phase diagram and in the compensation temperatures of the mixed spin-3/2 and spin-2 Ising ferrimagnetic system. The existence of the compensation temperatures in ferrimagnets has an interesting application such as the magneto-optical recording [27].

The outline of this work is as follows. In Section 2 we define the model and present the mean-field theory based on Bogoliubov inequality for the Gibbs free energy. We also have described Landau expansion of the free energy in the ordered parameter. In Section 3 we discuss the phase diagrams and compensation temperature for various values of the single ion anisotropies. Finally, In Section 4 we present our conclusions.

2. Model and Formulation

The model we investigate is the mixed spin-3/2 and spin-2 Ising ferrimagnetic system described by the Hamiltonian

$$H = -J\sum_{i,j} S_i^A S_j^B - D_A \sum_{i=1}^{N/2}\left(S_i^A\right)^2 - D_B \sum_{j=1}^{N/2}\left(S_j^B\right)^2, \quad (1)$$

where the first summation is carried out only over nearest neighbour pairs of spins on different sublattices and $J\ (J<0)$ is the nearest-neighbour exchange interaction. In this system, sites of the sublattice *A* are occupied by spins S_i^A, which take the values ± 1, ± 2 and 0 while those of the sublattice *B* are occupied by spins S_j^B, which take the values $\pm 1/2$ and $\pm 3/2$. D_A is the crystal field interaction constant of spin-2 ions and D_B is that of spin-3/2 ions. In order to treat the model approximately we employ a variational method based on the Bogoliubov inequality for the Gibbs free energy which is given by:

$$G(H) \le G_0(H_0) + \langle H - H_0\rangle_0 \equiv \phi, \quad (2)$$

where $G(H)$ is the true free energy of the system described by the Hamiltonian (1), $G_0(H)$ is the average free energy of a trial Hamiltonian H_0 and $\langle\ \rangle_0$ denotes a thermal average over the ensemble defined by H_0.

To obtain the *MFA*, we assume the trial Hamiltonian in the form

$$\begin{aligned} H_o = &-\sum_i\left[\gamma_A S_i^A + D_A\left(S_i^A\right)^2\right] \\ &-\sum_j\left[\gamma_B S_j^B + D_B\left(S_j^B\right)^2\right], \end{aligned} \quad (3)$$

where γ_A and γ_B are the two variational parameters related the molecular fields acting on the two different spins, respectively. Already at this stage it is clear that the use of the trial Hamiltonian (3) naturally leads to the mean-field approximation for the present model. Because of the simplicity of H_0, it is easy to evaluate the expressions in Equation (3) and we finally obtain

$$\begin{aligned} g \equiv \frac{\phi}{N} = \frac{1}{2\beta}\Big\{&\ln\left[2\exp(4\beta D_A)\cosh(2\beta\gamma_A) + \exp(\beta D_A)\cosh(\beta\gamma_A) + 1\right] \\ &+ \ln\left[2\exp(9\beta D_B/4)\cosh(3\beta\gamma_B/2) + 2\exp(\beta D_B/4)\cosh(\beta\gamma_B/2)\right]\Big\} \\ &+ \frac{1}{2}\left[-zJm_Am_B + \gamma_A m_A + \gamma_B m_B\right], \end{aligned} \quad (4)$$

where: $\beta = 1/k_BT$, *N* is the total number of sites of the lattice and *z* is the number of the nearest neighbors of every ion in the lattice. m_A and m_B are the sublattice magnetizations per site which defined by

$$m_A = \frac{4\sinh(2\beta\gamma_A) + 2\exp(-3\beta D_A)\sinh(\beta\gamma_A)}{2\cos(2\beta\gamma_A) + 2\exp(-3\beta D_A)\cosh(\beta\gamma_A) + \exp(-4\beta D_A)}, \quad (5)$$

$$m_B = \frac{3\sinh(3/2\,\beta\gamma_B) + \exp(-2\beta D_B)\sinh(1/2\,\beta\gamma_B)}{2\cosh(3/2\,\beta\gamma_B) + 2\exp(-2\beta D_B)\cosh(1/2\,\beta\gamma_B)}, \quad (6)$$

Now, by minimizing the free energy (4) with respect to γ_A and γ_B, we determine these parameters in the form

$$\gamma_A = zJm_B, \quad \gamma_B = zJm_A, \quad (7)$$

The mean field properties of the present system are then given by Equations (4)-(7). As the set of Equations (5)-(7) have in general several solutions for the pair (m_A, m_B), and the pair chosen is that which minimizes the free energy in Equation (4). So, analysis of the phase diagrams must be performed numerically. Nevertheless, some parts of the phase diagrams must be discussed analytically. For instance, close to the second-order phase transition from the ordered state $(m_A \ne 0, m_B \ne 0)$ to the paramagnetic one $(m_A = m_B = 0)$, the sublattice magnetizations m_A and m_B are very small in the neighborhood of second-order transition point, so, we may expand Equations (4)-(6) to obtain a Landau-like expansion in the form

$$g = g_0 + am_A^2 + bm_A^4 + cm_A^6 + O\left(m_A^8\right), \quad (8)$$

where the coefficients a and b are given by

$$a = a_1\left(8b_1t^2\left(4.5+0.5X_B\right) + 2b_1X_At^2\left(4.5+0.5X_B\right)\right) \quad (9)$$

$$\begin{aligned} b = a_1\Big(&1.3333t^4b_1^3\left(-81-67X_B+13X_B^2-X_B^3\right. \\ &\left.+364.5t^2+121.5t^2X_B+13.5t^2X_B^2+0.5t^2X_B^3\right) \\ &+0.6666t^4X_Ab_1^3\left(-40.5-33.5X_B+6.5X_B^2\right. \\ &-0.5X_B^3+45.5625t^2+15.1875t^2X_B+1.6875t^2X_B^2 \\ &\left.+0.0625t^2X_B^3\right)-a_1b_1\left(\left(8+2X_A\right)t^2\left(4.5+0.5X_B\right)\right. \\ &\left.\times\left(4t^4b_1^2\left(4.5+0.5X_B\right)^2+t^4b_1^2X_A\left(4.5+0.5X_B\right)^2\right)\right)\Big), \end{aligned} \quad (10)$$

where

$$t = \beta zJ,\ X_A = \exp\left(-3\beta D_A\right),\ X_B = \exp\left(-2\beta D_A\right),$$

$$a_1 = \frac{1}{2+2X_A},\quad b_1 = \frac{1}{2+2X_B}.$$

For simplicity, the coefficient c is not given here. In this way, we can obtain second-order phase transition lines when $a = 0$ and $b > 0$; and tricritical points when $a = b = 0$ and $c < 0$. It should be noted that the coefficients a and b are even functions of J. Therefore, the critical behaviour is the same for both ferromagnetic ($J > 0$) and ferrimagnetic ($J < 0$) systems. On the other hand, in the ferrimagnetic case the signs of sublattice magnetizations are different, and there may be compensation temperature $T_k\left(T_k < T_c\right)$ at which the total magnetization per site M is equal to zero, although $m_A \neq 0$ and $m_B \neq 0$. We are here interested in studying the phase diagrams and the compensation temperature, if it exists, in the system which can be determined from the equation

$$M = \frac{1}{2}\left(m_A + m_B\right) \quad (11)$$

3. Results and Discussions

3.1. The Ground-State Phase Diagram

Before going into detailed calculation of the phase diagram of the model at higher temperature, we begin with the ground-state structure of the system at zero temperature analytically. The ground-state phase diagram is easily found from Hamiltonian (1) by comparing the ground-state energies of different phases, and is shown in **Figure 1**. The ground state energy configurations is the one with the lowest energy and each of these configurations for the given system parameters correspond to the stable states of the model. Hence, at zero temperature, we find four phases with Different values of $\left\{m_A, m_B, q_A, q_B\right\}$, namely the ordered phases.

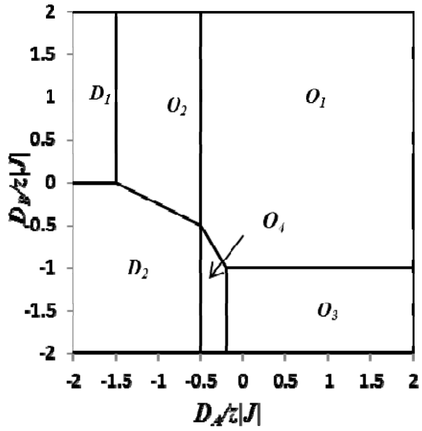


Figure 1. Ground-state phase diagram of a mixed spin-3/2 and spin-2 Ising ferrimagnetic system with the coordination number z and different single-ion anisotropies D_A and D_B. The six phases: ordered O_1, O_2, O_3, O_4 and disordered D_1, D_2 are separated by lines of first-order transitions.

These ordered phase are $O_1 = \left\{-2, 3/2, 4, 9/4\right\}$ (or $\left\{2, -3/2, 4, 9/4\right\}$ as well), $O_2 = \left\{-1, 3/2, 1, 9/4\right\}$ (or $\left\{1, -3/2, 4, 9/4\right\}$ as well), $O_3 = \left\{-2, 1/2, 4, 1/4\right\}$ (or $\left\{2, -1/2, 4, 1/4\right\}$ as well), $O_4 = \left\{1, -1/2, 1, 1/4\right\}$ (or $\left\{-1, 1/2, 1, 1/4\right\}$ as well), and disordered phases $D_1 = \left\{0, 0, 0, 9/4\right\}$ $D_2 = \left\{0, 0, 0, 1/4\right\}$, where the parameter q_A and q_B are defined by:

$$q_A = \left\langle\left(S_i^A\right)^2\right\rangle,\ q_B = \left\langle\left(S_j^B\right)^2\right\rangle.$$

3.2. The Finite Temperature Phase Diagrams

For the finite temperature phase diagrams, we have confined our calculations only to the second-order phase including the tricritical points. The resulting phase diagram in the $\left(D_A/z|J|, k_BT/z|J|\right)$ plane, for selected values of $\left(D_B/z|J|\right)$ is shown in **Figure 2**.

In this Figure, the solid lines are used to represent the second-order transitions, while the dashed curve represents the positions of tricritical points (The critical points at which the phase transitions change from second to first-order). The second-order phase transition lines are obtained from Equations (9) and (10) by setting $a = 0$ and $b > 0$ and the tricritical points are obtained from Equations (9) and (10) by setting $a = b = 0$. In particular, the values of the transition temperature in the absence of anisotropies (*i.e.* for $\left(D_A = D_B = 0\right)$ are $k_BT_c/z|J| =$ 1.5812. Furthermore, from **Figure 2**, we note that in regions of high temperatures, for all positive and negative values of $\left(D_B/z|J|\right)$, and for any value of $\left(D_A/z|J|\right)$, the phase diagram shows only second-order phase transitions. We also found that for values of $\left(D_B/z|J|\right) \geq 1.85$ all the second-order lines end in the same tricritical point

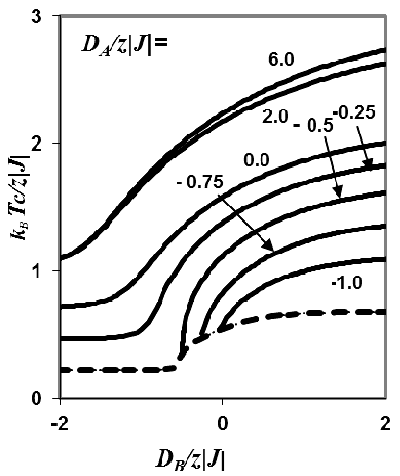


Figure 2. Phase diagram in the (D_A, T) plane for the mixed-spin Ising ferrimagnet with the coordination number z, when the value of $D_A/z|J|$ is changed. The solid lines indicate second-order phase transitions and the dashed line represents the positions of tricritical points.

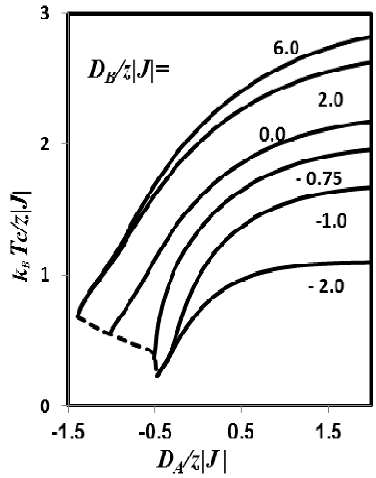


Figure 3. Phase diagram in the (D_B, T) plane for the mixed-spin Ising ferrimagnet with the coordination number z, when the value of $D_A/z|J|$ is changed. The solid lines indicate second-order phase transitions and the dashed line represents the positions of tricritical points.

given by $\left(D_A/z|J|\right) = -1.3955$ and $k_BT_c/z|J| = 0.6782$. However, for values of $\left(D_B/z|J|\right) \le -1.15$, all the second-order lines end in the same tricritical point given by $\left(D_A/z|J|\right) = -0.466$ and $k_BT_c/z|J| = 0.2264$. Additionally, the diagram shows that when the coordinates $\left(D_A/z|J|, k_BT_{3c}/z|J|\right)$ of the tricritical point are $(-1.3955, 0.6782)$ the mixed spin Ising system behaves like a two level system since the spin-3/2 behaves like $S_j^B = \pm 3/2$. On the other hand, for $D_B \to -\infty$, the coordinates $\left(D_A/z|J|, k_BT_c/z|J|\right)$ of the tricritical point are $(-0.4660, 0.2264)$. In this case, the states $S_j^B = \pm 3/2$ are suppressed and the system becomes equivalent to a mixed spin-1/2 and spin-2 Ising model. For this reason, the coordinates of the tricritical point in the limit of large positive D_B are three times higher than those for large negative D_B.

In **Figure 3**, it is shown the phase diagram of $k_BT_c/z|J|$ versus $D_B/z|J|$ for various values of $D_A/z|J|$. For $D_A/z|J| > -0.4660$ the phase diagrams are topologically equivalent to phase diagram for the spin-3/2 Blume-Capel model which does not include any tricritical point. From **Figure 3**, one can observe the variation of the tricritical temperature with $D_B/z|J|$. The Tricritical temperature $k_BT_{3c}/z|J|$ decreases from its constant value $k_BT_{3c}/z|J| = 0.6782$ for large positive $D_B/z|J|$ to another constant value $k_BT_{3c}/z|J| = 0.2264$ for large negative $D_B/z|J|$.

3.3. Compensation Temperatures

A compensation temperature of the system can be evaluated by requiring the condition $M = 0$ in the coupled Equations (4) and (5).

Now, let us investigate whether the present mixed-spin Ising ferrimagnetic system may exhibit a compensation point (or points) at $T \ne 0$ when the single-ion anisotropies are changed. The variation of the compensation temperature T_k as a function of $D_A/z|J|$ for different values of $D_B/z|J|$ is shown in **Figure 4**.

As seen from **Figures 4(a)** and **(b)**, all the curves emerge from the point $D_A/z|J| = -0.5$ at $T = 0\ K$ and exhibit some characteristic behaviours when the value of $D_B/z|J|$ is controlled.

By selecting the appropriate values of $D_B/z|J|$ and. as $D_B/z|J|$ is reduced, the range of $D_A/z|J|$ over which the compensation points occurs gradually becomes small, but the compensation temperature still reaches the corresponding transition line.

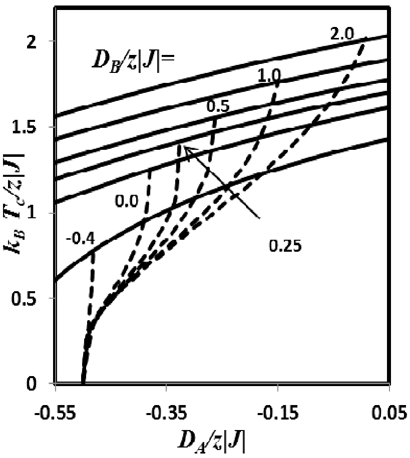
When the values of $D_B/z|J| \ge -0.4$ are selected (**Figure 4(a)**) the curves increase monotonically with $D_A/z|J|$ to terminate at the corresponding phase boundaries (solid lines).

As shown in **Figure 4(b)**, in a restricted region of $D_B/z|J|$, close to $D_B/z|J| = -0.5$, the compensation temperature curves exhibit bulges, which implies the occurrence of two and three compensation points in the system.

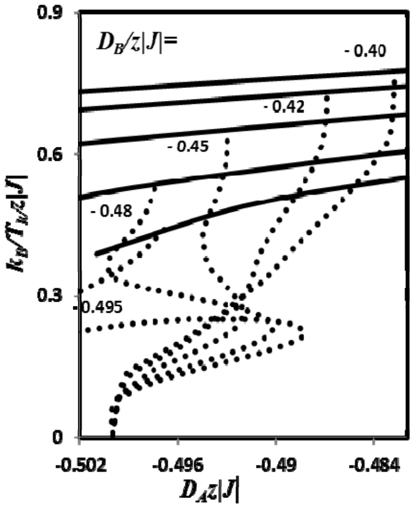
Typical sublattice magnetization curves, with one compensation point, two compensation points and three compensation points are shown in **Figures 5(a)-(c)**, respectively, for selected values of $D_A/z|J|$ and $D_B/z|J|$. It is easy to see that these compensation points in the magnetization curves are in agreement with the compensation points given in **Figure 4**.

4. Conclusion

In this paper, we have determined the global phase dia-



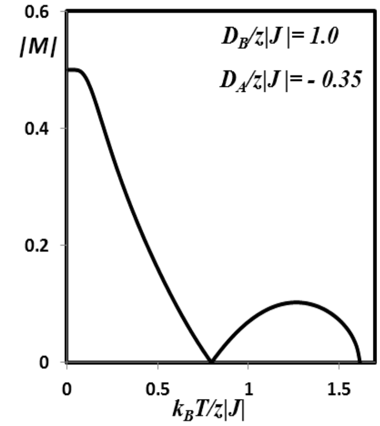
(a)



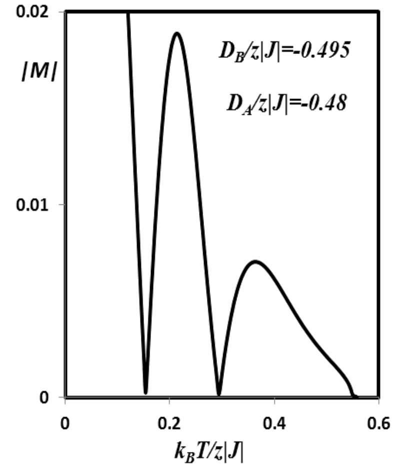
(b)

Figure 4. Dependence of the compensation temperature (dotted curves) on the single-ion anisotropy. $D_A/z|J|$ in a mixed-spin Ising ferrimagnet with the coordination number z, when the value of $D_B/z|J|$ is changed. (a) The curves show the positions of one compensation points only; (b) The curves show the positions of one, two and three compensation points. The solid curves represent the second-order transitions.

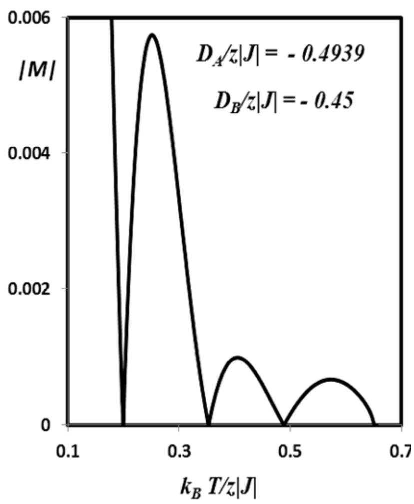
grams of the mixed spin-3/2 and spin-2 Ising ferrimagnetic system with different single-ion anisotropies acting on the spin-3/2 and spin-2 by using mean-field approximation. In the phase diagrams, the critical temperature lines versus single-ion anisotropies are shown. The system presents tricritical behaviour, *i.e.*, the second-order phase transition line is separated from the first-order transition line by a tricritical point. We also observed that this mixed-spin ferrimagnetic system may exhibit one, two or three compensation points. The theoretical prediction of the possibility of compensation points and the design and preparation of materials with such unusual behaviour will certainly open a new area of research on



(a)



(b)



(c)

Figure 5. Thermal variations of the total magnetization |M| for the mixed-spin Ising ferrimagnet with the coordination number z. (a) When the value of $D_B/z|J| = 1.0$ and $D_A/z|J| = -0.35$ (to show one compensation point); (b) When the value of $D_B/z|J| = -0.48$ and $D_A/z|J| = -0.495$ (to show two compensation points); (c) When the value of $D_B/z|J| = -0.45$ and $D_A/z|J| = -0.4939$ (to show three compensation points).

such materials.

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