

The possibility of four compensation points in a mixed spin-2 and spin-7/2 Ising ferrimagnetic system using mean-field theory

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Abstract

The compensation points of this mixed spin ferrimagnetic system are examined by the use of the mean-field theory based on Bogoliubov inequality for the free energy. The ground-state phase diagram is constructed in order to show the first order transition lines separating the ordered and the disordered phases of the system at zero temperature. The influence of the single-ion anisotropies D_A and D_B , on the compensation points is studied in detail. The model exhibits up to four compensation temperatures for appropriate values of the single-ion anisotropies.

Keywords: *Compensation points; Mean field theory; Total magnetization; Sublattice magnetization; Mixed-spin Ising model; Ferrimagnet; Single ion anisotropy.*

1. Introduction

Over recent years there has been considerable interest in the study of two sublattice mixed-spin Ising ferrimagnetic systems. The mixed-spin Ising systems in comparison with the systems with one type of spins present less translational symmetry and a new type of critical temperature called a compensation temperature T_K appears. The compensation temperature is a temperature which below the critical temperature, T_c , and at which the sublattice magnetizations compensate each other and the resultant magnetization vanishes [1]. Some compensation temperature points were obtained experimentally in Fe_3O_4 and Mn_3O_4 super lattices [2], From the experimental point of view, previous studies show that at the compensation temperature, the coercivity of a material increases dramatically and at this point only a small conductor field is required to invert the sign of the magnetization [3–6]. Furthermore, the two sublattice mixed-spin ferrimagnetic systems are proposed to describe a certain type of molecular-based magnetic materials. These types of magnetic materials are studied experimentally [7-10] and the researches in these ferrimagnetic materials are of great interests due to their possible technological applications, especially in the magneto-optical recording [11, 12]. Zaim and Kerouad [13] indicated that mixed Ising spin models are useful models in industrial applications of emerging nanotechnology, which can be used for a variety of nano-devices, due to their reduced size and important magnetic properties such as high density magnetic memories, sensors and molecular imaging devices, etc. The existence of the compensation temperature points in the mixed-spin-1 and spin-3/2 Ising ferrimagnetic system and the influence of the crystal field (single ion anisotropies) or the transverse field on these compensation points was examined by various methods e.g. the mean-field approximation [14], the effective-field theory with correlations [15-20], the cluster variational method with the pair approximation [21], the Beth lattice solution [22-23], and Monte Carlo simulation [24]. All of these methods indicate the existence of the compensation points in the system. The attention was devoted to the high order mixed spin ferrimagnetic systems and the compensation temperature points were found by using various methods. e.g. the critical and compensation temperatures for the mixed spin-3/2 and spin-5/2 [25], the mixed spin-3/2 and spin-2 [26] and the mixed spin-2 and spin-5/2 [27] Ising ferrimagnetic systems, on the Bethe lattice, was investigated by using the exact recursion equations and all these Ising systems (by using this method) exhibit compensation temperature points. The effect of the single-ion anisotropies on the critical and the compensation points also investigated in the mixed spin-3/2 and spin-2 [28] and the mixed spin-2 and spin-5/2 [29] Ising ferrimagnetic systems by using the mean-field theory based on the Bogoliubov inequality for the free energy. Furthermore, the mixed spin-2 and spin-3/2 Blume-Emery-Griffiths (BEG) Ising ferrimagnetic system is studied by the Bethe lattice approach [30]. In this system, compensation points have been detected for appropriate values of the system parameters. Finally, Monte Carlo simulation was used to study the effect of an external magnetic field on a mixed-spin-3/2 and spin-5/2 Ising ferrimagnet and during the consideration, compensation points

were detected depending on the region of the parameter space [31]. In this paper, we extend the investigations to high order mixed spin ferrimagnetic system. The system we consider is the mixed spin-2 and the spin-7/2 ferrimagnetic system within the frame-work of the mean-field theory, in order to examine the existence of the compensation temperature points and to study the effects of the single-ion anisotropies of this system on the compensation temperature lines.

This work includes, in Section 2, a formulation of the model and its mean-field solution. In this section, we give a Landau expression of the free energy in the order parameters and we prepare the required Equations for the sublattice magnetizations m_A and m_B , the total magnetization M and the free energy F . In Section 3, we construct the ground state phase diagram, we plot and discuss the compensation temperature lines as a function of temperature and we discuss the thermal variation of the total and the sublattice magnetizations for various values of the anisotropies in order to assure the existence of the compensation temperature points, Finally, in Section 3 we present our conclusions.

2. Formulation of the model and its mean-field solution

The model we are going to consider, consists of two dimensional sublattices. The sublattice A with spin values $S_i^A = \pm 2, \pm 1, 0$ and the sublattice B with spin values $S_j^B = \pm 7/2, \pm 5/2, \pm 3/2, \pm 1/2$. This system is described by the following Hamiltonian:

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

In this Hamiltonian, the first summation is carried out only over nearest-neighbour pairs of spins on different sublattices and J is the exchange interaction between spins at sites i and j . D_A and D_B are the crystal-field interactions or the single-ion anisotropies acting on the spin S_j^B and spin S_j^B , respectively.

In order to solve this Hamiltonian approximately by using the mean-field solution, we employ a variational method based on the Bogoliubov inequality for the free energy [14], namely

$$F(\mathcal{H}) \leq \Phi \equiv F_0(\mathcal{H}_0) + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 \quad (2),$$

where \mathcal{H} is the Hamiltonian given by Eq (1) and $F(\mathcal{H})$ is the free energy of \mathcal{H} , \mathcal{H}_0 is a trial Hamiltonian depending on variational parameters and $F_0(\mathcal{H}_0)$ is the free energy of the trial Hamiltonian \mathcal{H}_0 . $\langle \dots \rangle_0$ denotes a thermal average over the ensemble defined by \mathcal{H}_0 .

To facilitate the calculations, we choose the simplest trial Hamiltonian, which is given by:

$$\mathcal{H}_0 = -\sum_i (\alpha_A S_i^A + D_A (S_i^A)^2) - \sum_j (\alpha_B S_j^B + D_B (S_j^B)^2) \quad (3)$$

Where α_A and α_B are the two variational parameters related to the two different spins.

By using \mathcal{H}_0 , we can find the free energy per site and the equations of state (sublattice magnetization per site m_A and m_B):

$$f \equiv \frac{\Phi}{N} \leq -\frac{1}{2\beta} \left(\ln \left(1 + \exp(4\beta D_A) (2 \cosh(2\beta \alpha_B) + 2A \cosh(\beta \alpha_B)) \right) + \ln \left(\begin{array}{l} 2 \exp\left(\frac{49\beta D_B}{4}\right) \cosh(3.5 \beta \alpha_A) \\ + 2 \exp\left(\frac{25\beta D_B}{4}\right) \cosh(2.5 \beta \alpha_A) \\ + 2 \exp\left(\frac{9\beta D_B}{4}\right) \cosh(1.5 \beta \alpha_A) \\ 2 \exp\left(\frac{\beta D_B}{4}\right) \cosh(0.5 \beta \alpha_A) \end{array} \right) \right) + \frac{1}{2} [-z] \langle S_i^A \rangle_0 \langle S_j^B \rangle_0 + \alpha_A \langle S_i^A \rangle_0 + \alpha_B \langle S_j^B \rangle_0, \quad (4)$$

where, N is the total number of sites of the lattice, z its coordination number and $\beta = 1/k_B T$. The averaged sublattice magnetizations per site defined as $m_A = \langle S_i^A \rangle_0$ and $m_B = \langle S_j^B \rangle_0$, where $\langle S_i^A \rangle_0$ and $\langle S_j^B \rangle_0$, indicate the thermal (configurational) average and are given by

$$m_A = \frac{4 \sinh(2\beta\alpha_B) + 2A \sinh(\beta\alpha_B)}{2 \cosh(2\beta\alpha_B) + 2A \cosh(\beta\alpha_B) + E} \tag{5}$$

$$m_B = \frac{7 \sinh(\frac{7}{2}\beta\alpha_A) + 5B \sinh(\frac{5}{2}\beta\alpha_A) + 3C \sinh(\frac{3}{2}\beta\alpha_A) + D \sinh(\frac{1}{2}\beta\alpha_A)}{2(\cosh(\frac{7}{2}\beta\alpha_A) + B \cosh(\frac{5}{2}\beta\alpha_A) + C \cosh(\frac{3}{2}\beta\alpha_A) + D \cosh(\frac{1}{2}\beta\alpha_A))} \tag{6}$$

where,

$$A = \exp(-3D_A/k_B T), E = \exp(-4D_A/k_B T), B = \exp(-6D_B/k_B T),$$

$$C = \exp(-10D_B/k_B T), D = \exp(-12D_B/k_B T).$$

We are here interested in studying the compensation temperature points, if they exist in the system, which can be determined when the total magnetization m vanishes. Therefore, we need equation for the total magnetization m , which is given by

$$M = \frac{m_A + m_B}{2} \tag{7}$$

By minimizing the free energy in terms of the variational parameters α_A and α_B , we have obtained

$$\alpha_A = Jz m_B, \quad \text{and} \quad \alpha_B = Jz m_A. \tag{8}$$

Eqs (4-8) are mean-field equations which provide the magnetic properties of the system under consideration. The equations (5-7) have several solutions for m_A and m_B and the stable solution is the one which gives the minimum free energy. So, the detailed phase diagram is determined and performed by numerical analyses. Since the magnetizations m_A and m_B are very small, close to the second-order phase transition where the system changes from ordered ferrimagnetic phase to disordered paramagnetic phase, we can expand the equations (5-6) to obtain a Landau-like expansion.

$$f = f_0 + a m_A^2 + b m_A^4 + m_A^6 + \dots \tag{9}$$

where the expansion coefficients are given by

$$f_0 = -\frac{1}{2\beta} \left(\ln(1 + 2\exp(4\beta D_A)) + \ln \left(\frac{2\exp(\frac{49\beta D_B}{4}) + 2\exp(\frac{25\beta D_B}{4})}{+2\exp(\frac{9\beta D_B}{4}) + 2\exp(\frac{\beta D_B}{4})} \right) \right), \tag{10}$$

$$a = \frac{\frac{49 t^2 (A + 4)}{2 + 2A + E} + \frac{25 B t^2 (A + 4)}{2 + 2A + E} + \frac{9 C t^2 (A + 4)}{2 + 2A + E} + \frac{D t^2 (A + 4)}{2 + 2A + E}}{2 + 2B + 2C + 2D} \tag{11}$$

$$\begin{aligned}
b = & \frac{1}{2+2B+2C+2D} \left(\left(\frac{49}{6} \frac{1}{(2+2A+E)^3} (t^4 (49A^3t^2 + 588A^2t^2 - 8A^3 - 2A^2E \right. \right. \\
& \left. \left. + AE^2 + 2352At^2 - 36A^2 + 20AE + 16E^2 + 3136t^2 - 156A - 32E - 128) \right) \right. \\
& \left. + \frac{25}{6} \frac{1}{(2+2A+E)^3} (Bt^4 (25A^3t^2 + 300A^2t^2 - 8A^3 - 2A^2E + AE^2 \right. \\
& \left. + 1200At^2 - 36A^2 + 20AE + 16E^2 + 1600t^2 - 156A - 32E - 128) \right) \\
& \left. + \frac{3}{2} \frac{1}{(2+2A+E)^3} (Ct^4 (9A^3t^2 + 108A^2t^2 - 8A^3 - 2A^2E + AE^2 + 432At^2 \right. \\
& \left. + \frac{1}{6} \frac{1}{(2+2A+E)^3} (Dt^4 (A^3t^2 + 12A^2t^2 - 8A^3 - 2A^2E + AE^2 + 48At^2 - 36A^2 \right. \\
& \left. + 20AE + 16E^2 + 64t^2 - 156A - 32E - 128) \right) \\
& - \frac{1}{2} \frac{1}{(2+2A+E)(1+B+C+D)} \left(t^2(A+4)(49+25B+9C \right. \\
& \left. + D) \left(\frac{49t^4(A+4)^2}{(2+2A+E)^2} + \frac{25Bt^4(A+4)^2}{(2+2A+E)^2} + \frac{9Ct^4(A+4)^2}{(2+2A+E)^2} \right. \right. \\
& \left. \left. + \frac{Dt^4(A+4)^2}{(2+2A+E)^2} \right) \right) \right) \tag{12}
\end{aligned}$$

Where, $t = \beta z$

From equations (11) and (12), it is clear that the coefficients a and b are even functions in J which means that the critical points have the same values for both ferromagnetic system (when $J>0$) and ferrimagnetic system (when $J<0$).

3. Results and discussions

3.1 Ground state Phase diagram

Before going into the detailed calculation of the phase diagram of the present system at higher temperatures, the ground-state phase diagram (see Fig. 1) is determined by comparing the energies given in the Hamiltonian (1) of different phases at zero temperature. As shown in this figure, the structure of the ground state of the system consists of eight ordered ferrimagnetic phases and four disordered phases, separated by first ordered lines, and these phases have different values of $\{m_A, m_B, q_A, q_B\}$

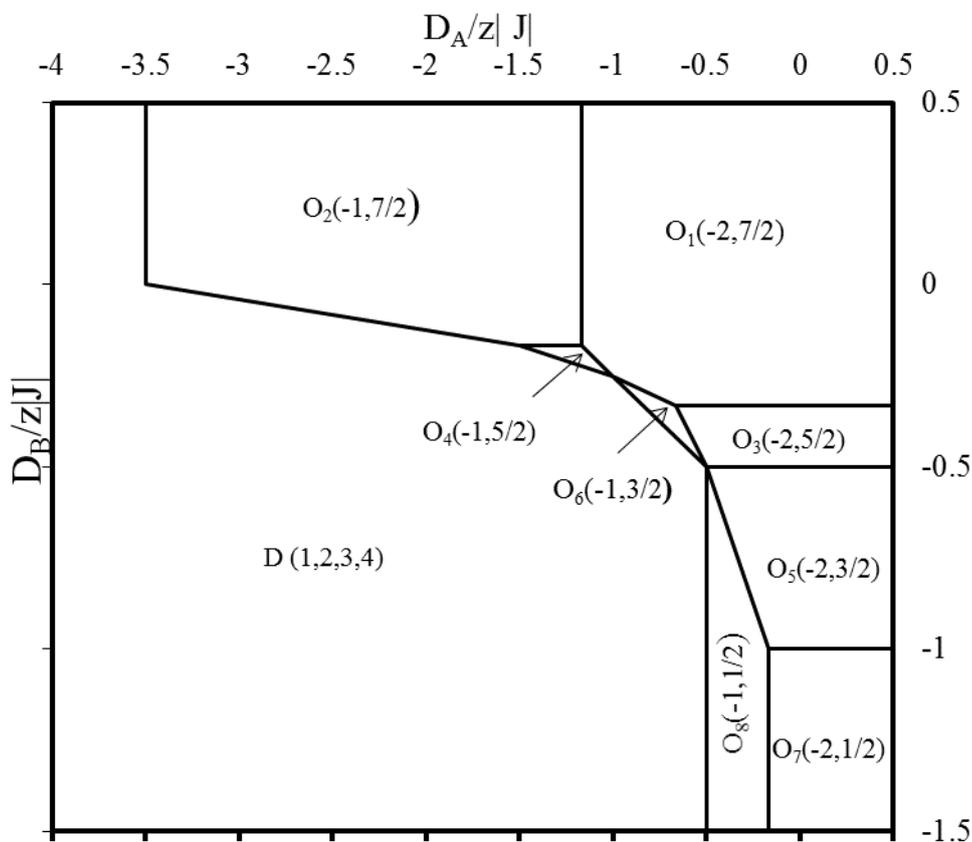


Fig. 1: Ground-state phase diagram of the mixed spin-2 and spin-7/2 Ising ferrimagnetic system on the $(D_A/z|J|, D_B/z|J|)$ plane. In this phase diagram, there are eight ordered phases $O_1, O_2, O_3, O_4, O_5, O_6, O_7$ and O_8 , and four disordered phases D_1, D_2, D_3 and D_4 .

The values $\{m_A, m_B, q_A, q_B\}$ for the ordered phases are given as following:

$$O_1 = \left\{-2, \frac{7}{2}, 4, \frac{49}{4}\right\}, \quad O_2 = \left\{-1, \frac{7}{2}, 1, \frac{49}{4}\right\}, \quad O_3 = \left\{-2, \frac{5}{2}, 4, \frac{25}{4}\right\},$$

$$O_4 = \left\{-1, \frac{5}{2}, 1, \frac{25}{4}\right\}, \quad O_5 = \left\{-2, \frac{3}{2}, 4, \frac{9}{4}\right\}, \quad O_6 = \left\{-1, \frac{3}{2}, 1, \frac{9}{4}\right\}$$

$$O_7 = \left\{-2, \frac{1}{2}, 4, \frac{1}{4}\right\}, \quad O_8 = \left\{-1, \frac{1}{2}, 1, \frac{1}{4}\right\},$$

and for the disordered phases are given as following:

$$D_1 = \left\{0,0,0, \frac{49}{4}\right\}, \quad D_2 = \left\{0,0,0, \frac{25}{4}\right\}, \quad D_3 = \left\{0,0,0, \frac{9}{4}\right\}, \quad D_4 = \left\{0,0,0, \frac{1}{4}\right\}.$$

3.2 Compensation temperature points

The compensation temperature T_k is the temperature where the resultant magnetization vanishes below the critical temperature. In this subsection, we will investigate whether the present mixed-spin Ising ferrimagnetic system may exhibit a compensation point (or points) at $T \neq 0$ when the single-ion anisotropies are changed. The compensation temperature T_k , if it exists in the system, can be determined from the condition that the total magnetization M in equation (7) vanishes ($M=0$) below its transition

temperature T_c . In Fig. 2 (a) and (b), the diagram $k_B T_c / z|J|$ and $k_B T_k / z|J|$ versus $D_B / z|J|$ are shown for some selected values of $D_A / z|J|$. In these two figures, the solid lines represent a part of the second-order transition lines separating the paramagnetic and ferrimagnetic phases. These lines were obtained numerically by following this routine: 1) When $a=0$ and $b>0$, the lines will be second order transition lines. 2) When $a=0$ and $b=0$, the points determine the tricritical points. 3) By comparing the free energy f given in eq (4) with f_0 given in eq (10), the first order transition lines (dashed line in the figure) can be determined when $f = f_0$.

As can be seen from figure 2 (a), when the selected values of $D_A / z|J|$ are $D_A / z|J| = 5.0, 1.0, 0.5, 0.0, 0.3$, all the T_k curves emerge from the same point $D_A / z|J| = -0.5$ at $T = 0K$, increase monotonically and terminate at the corresponding phase boundaries. The monotonical behavior of the curves indicates that only one compensation point may occur in this mixed spin ferrimagnetic system. It is clear from this figure also that as the values of $D_A / z|J|$ is increased, the intersection of the T_k curves with the T_c curves is moved to higher values of $k_B T_c / z|J|$. In figure.2 (b), when the values of $D_A / z|J|$ are selected to have the values $D_A / z|J| = -0.45, -0.47, -0.495, -0.499$, a new type of compensation curves appear. In this values of $D_A / z|J|$, the curves of T_k , for a small range of $D_B / z|J|$, exhibit a non-monotonical behavior, such as the dotted curve for $D_A / z|J| = -0.499$. It indicates that two, three or even four compensation points may occur, below the critical points, in this mixed-spin system. From this figure, it is clear that the system exhibits this interesting behavior in the points close to the point $(D_A / z|J|, D_B / z|J|) = (-0.5, -0.5)$ in the ground-state phase diagram.

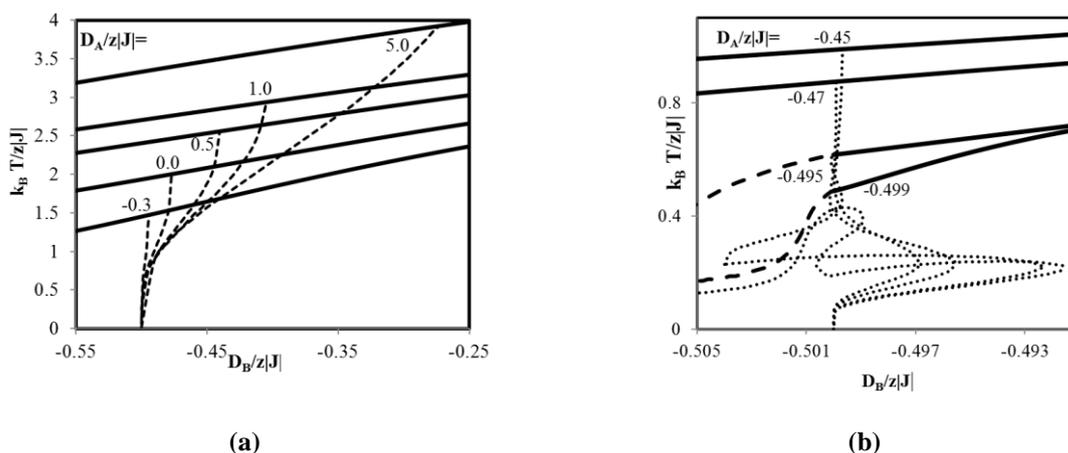


Fig. 2 The compensation points (dotted curves) versus the single-ion anisotropy $D_B / z|J|$ for some selected values of the single-ion anisotropy $D_A / z|J|$. (a) The curves show the positions of one compensation points only; (b) The curves show the positions of one, two, three and four compensation points. The solid and dashed curves represent the second-order and first-order transitions respectively

3.3 Total and sublattice magnetizations

Now, in order to confirm the existence of many compensation points, let us examine the total magnetization M as a function of temperature T . The total magnetization M versus T is plotted in the figures. 3.(a, b, c, d) for different values of $D_A / z|J|$ and $D_B / z|J|$ which chosen to locate on the region of the compensation curves shown in the figures 2.(a, b). In the figure. 3(a), one can see that the thermal variation of M exhibits one compensation point below the critical point T_c when the values of the single-ion anisotropies are chosen to be as $D_A / z|J| = 1.0$ and $D_B / z|J| = -0.45$. while, it exhibits two compensation points when $D_A / z|J| = -0.47$ and $D_B / z|J| = -0.499$, as can be seen in the figure 3(b). Furthermore, it is clear that when $D_A / z|J| = -0.499$, the system exhibits three and four compensation points when $D_B / z|J| = -0.5002$ and -0.4992 , respectively, as shown in figures 3(a) and 3(b). These results clearly express that the existence of one, two, three, or four compensation points shown in figures 2. (a, b) is correctly reproduced in the thermal variations of the total magnetization M . From these four figures, it can be observed that

the magnitude of the total magnetization between the last compensation point and the critical temperature point is always smaller than that between any two compensation points.

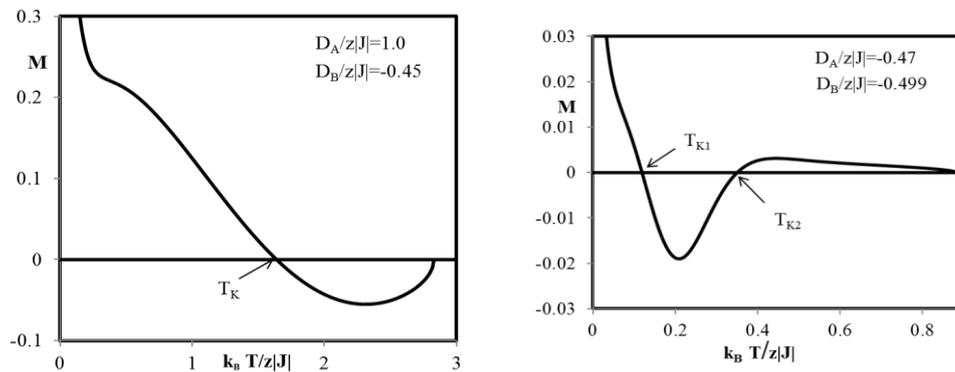


Fig. 3 (a, b) The thermal dependences of the total magnetization M for the mixed spin-2 and spin-7/2 Ising ferrimagnetic system with $z=1.0$ (a) when $D_A/z|J|=1.0$ and $D_B/z|J|=-0.45$. (b) when $D_A/z|J|=-0.47$ and $D_B/z|J|=-0.499$.

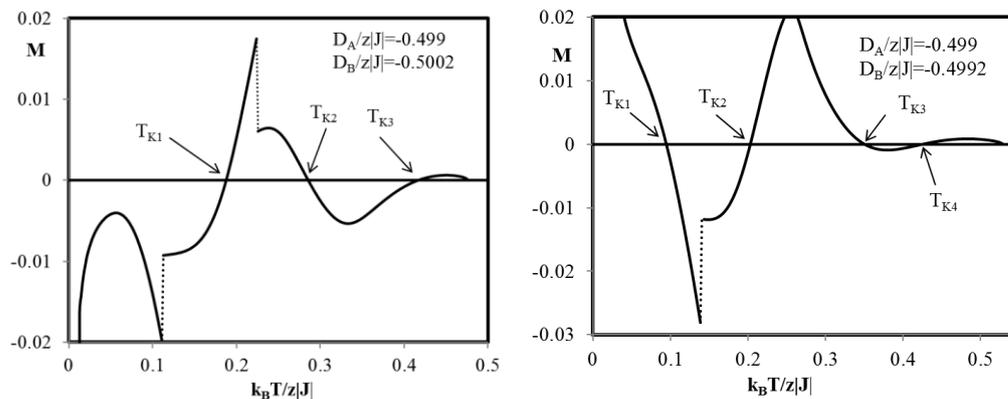


Fig. 3 (c, d) The thermal dependences of the total magnetization M for the mixed spin-2 and spin-7/2 Ising ferrimagnetic system with $z=1.0$ (a) when $D_A/z|J|=-0.499$ and $D_B/z|J|=-0.5002$. (b) when $D_A/z|J|=-0.499$ and $D_B/z|J|=-0.4992$.

Finally, in order to explain the reason for the occurrence of the compensation points in this mixed-spin ferrimagnetic system, we plot four curves which represent the variation of the absolute values of the sublattice magnetizations m_A and m_B with temperature at selected values of $D_A/z|J|$ and $D_B/z|J|$. These curves are shown in the figures 4(a - d) with the same values of $D_A/z|J|$ and $D_B/z|J|$, used in the figures 3(a - d), respectively. In fig.4(a), when $D_A/z|J|=1.0$ and $D_B/z|J|=-0.45$, the absolute values of the sublattice magnetizations $|m_A|$ and $|m_B|$ take the saturation values $|m_A|=2.0$ and $|m_B|=5/2$ at $T=0K$, in agreement with the ground-state phase diagram, (see Fig. 1). As the temperature increases, the sublattice magnetizations decreases and in the low-temperature region we have $|m_B|>|m_A|$ but in this region, $|m_B|$ exhibits a rapid decrease, while m_A exhibits a slow decrease and has a convex shape, as shown in Fig. 4(a), and they intersect each other at the compensation point T_K . As the temperature further increases, the values of $|m_A|$ becomes greater than the values of $|m_B|$ and they decrease by increasing the temperature until they vanish at the transition temperature T_c . In fig 4(b), when $D_A/z|J|=-0.47$ and $D_B/z|J|=-0.499$, as the temperature increases to values greater than the first compensation point T_{K1} , where $|m_A|>|m_B|$, the sublattice magnetization $|m_A|$ may be reduced below the sublattice magnetization $|m_B|$, before they fall to zero at the transition point T_c .

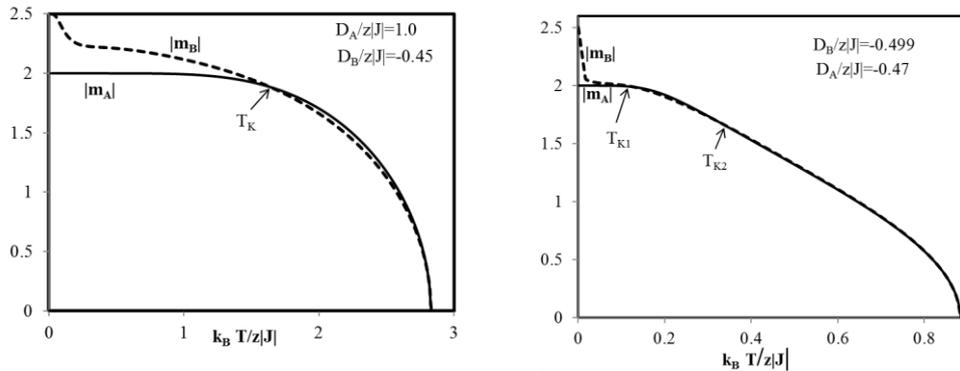


Fig. 4(a, b). The thermal variation of the absolute values of the sublattice magnetizations $|m_A|$ and $|m_B|$ for the mixed spin-2 and spin-7/2 Ising ferrimagnetic system (a) when $D_A/z|J|=1.0$ and $D_B/z|J|=-0.45$. (b) when $D_A/z|J|=-0.47$ and $D_B/z|J|=-0.499$.

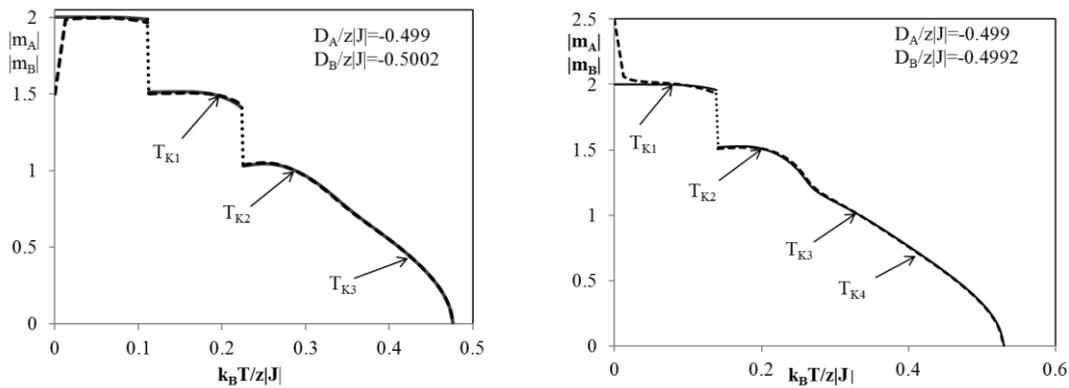


Fig. 4 (c, d) The thermal variation of the absolute values of the sublattice magnetizations $|m_A|$ and $|m_B|$ for the mixed spin-2 and spin-7/2 Ising ferrimagnetic system (a) when $D_A/z|J|=-0.499$ and $D_B/z|J|=-0.5002$. (b) when $D_A/z|J|=-0.499$ and $D_B/z|J|=-0.4992$.

As a result, an additional intersection between the two curves of the sublattice magnetizations may appear at a high temperature and cause the appearance of the second compensation point T_{K2} as shown in figures. 3(b) and 4(b). The last behaviour of the sublattice magnetization may occur three or four times to cause three points of intersection below the critical point when $D_A/z|J|= -0.47$ and $D_B/z|J|= -0.499$, as shown in fig. 4(c) or four points of intersection, when $D_A/z|J|= -0.47$ and $D_B/z|J|= -0.499$, as shown in figure. 4(d). As a result, this mixed spin system may exhibit three and four compensation points, as shown in fig.3 (c) and 3(d), respectively.

4. Conclusions

In this paper, we have used the mean-field theory based on Bogoliubov inequality for the Gibbs free energy to study the effects of two different anisotropies on the compensation temperature of the mixed spin-2 and spin-7/2 ferrimagnetic Ising system. The compensation temperature lines versus the single-ion anisotropy D_B (acting on the spin -2,) at selected values of the single-ion anisotropy D_A (acting on the spin-7/2) are shown. Our study suggests that there is a strong dependence between the compensation temperature and the single-ion anisotropies D_A and D_B : From the compensation lines, we have shown that this mixed spin system may exhibit one, two, three or even four compensation points. We found also that the system may show some interesting behaviour in the total and sublattice magnetizations (see

Fig.3(c) and 4(d)). These results can be compared with the results appeared in the literature [28], [29], [30]. Finally, we suggest that it will be very interesting to check the existence of the compensation points by more reliable techniques such as renormalization-group approach or Monte-Carlo simulation, and we believe that the design and preparation of ferrimagnetic materials with such unusual behaviour (compensation points) will certainly open a new area of research on such materials.

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