COMPENSATION TEMPERATURES OF MIXED SPIN-3/2 AND SPIN-5/2 FERRIMAGNETIC SYSTEM

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ABSTRACT

Compensation points of The mixed spin-3/2 and spin-5/2 Ising ferrimagnetic system with different sublattice crystal- fields is studied within the mean-field theory based on Bogoliubov inequality for the Gibbs free energy. In order to clarify the characteristic behaviours in a series of molecular-based magnets, for example, the molecular magnetic material $Cs_2Mn^{II}[V^{II}(CN)_6]$. The influence of two sublattice crystal fields, D_A and D_B, on compensation points is studied in detail. For certain crystal-field values, this mixed-spin model exhibits one, two or three compensation temperature depending on the values of the crystal-fields.

Keywords:Sublattice magnetization, Total magnetization, Mixed-spin Ising model, Ferrimagnet, Single-ion anisotropy, Compensation point**.**

1. INTRODUCTION

The two-sublattice mixed Ising ferrimagnetic systems have been of interest for not only purely theoretical purpose, but also they have been proposed as possible models to describe a certain type of molecular-based magnetic materials that are studied experimentally [1-4]. These materials are important magnetic materials for technology of thermo-magnetic recording [5-8]. Furthermore, 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 as a compensation temperature T_K, below the critical temperature (T_k< Tc), at which the resultant magnetization vanishes [9]. The occurrence of a compensation point has great technological importance, since at this point only a small driving field is required to change the sign of the resultant magnetization. This property is very useful in thermomagnetic recording. At the compensation temperature T_k, the coercivity of the material increases dramatically facilitating the process of writing and erasing in magneto-optical media [10]. The critical phenomena of the mixed spin-1 and spin-3/2 Ising model, which takes into account the influence of a crystal field or transverse field was examined by various methods, e.g., the effective-field theory with correlations (EFT) [11–16], the cluster variation method with the pair approximation (CVMPA) [17], the mean-field approximation (MFA) [18] and the Bethe lattice solution [19,20]. Some of them indicate the existence of the compensation points in the system. Recently, these investigations have been extended to high order mixed spin ferrimagnetic systems in order to study their magnetic properties. F. Abubrig studied the mixed spin-3/2 and spin-2 [21] andthe mixed spin-2 and spin-5/2 [22] Ising ferrimagnetic systemwith different single-ion anisotropiesby using the mean-field theory based on the Bogoliubov inequality, and he investigated the existence of the compensation points in the system. By means of exact recursion equations, Albayrak [23, 24] investigated the magnetic properties (Including the compensation points) of the mixed spin-2 and spin-3/2 and the mixed-spin-2 and spin-5/2 Blume Capel (BC) Ising model with different crystal-fields on the Bethe lattice]. Deviren *et al*. [25] used the effective field-theory to study the magnetic properties of the ferrimagnetic mixed spin-2 and spin-3/2 BC Ising model with equal crystal-field in a longitudinal magnetic field on the honeycomb and a square lattice and got interesting results [26].Furthermore**,** The mixed spin-2 and spin-3/2 Blume-Emery-Griffiths (BEG) Ising ferrimagnetic system is studied by the Bethe lattice approach [27].In this system, compensation points where the global magnetization of the system vanishes have been detected for appropriate values of the system parameters investigated. A ferrimagnetic mixed spin-3/2 and spin-5/2 Ising model with different crystal-fields is investigated.by Hadey K. Mohamad [28]. The results of this model predict the existence of many (two or three) compensation points in the ordered system on a simple cubic lattice. Finally, The magnetic properties of the mixed spin-3/2 and sin-5/2 Ising ferrimagnet are studied by Monte Carlo simulation [29]. During the consideration and depending on the region of the parameter space, compensation temperature points were found in this system.

In this paper, we studied the effects of two different crystal-fields on the compensation temperatures of the mixed spin-3/2 and spin- 5/2 Ising ferrimagnetic system within the theoretical frame- work of the mean-field theory.

The outline of this work is as follows. In Section 2, we define the model and present the mean-field theory based on the Bogoliubov inequality for the Gibbs free energy and we prepare the required Eqs for the sublattice magnetizations m_A and m_B, the total magnetization M and the free energy F. In Section 3, we present the results and the discussion about the compensation temperature for various values of the crystal-field constants , as well as the temperature dependences of the magnetizations in some particular cases. Finally, in Section 4, The conclusions are presented.

2. THE MODEL AND CALCULATION

We consider a mixed Ising spin-2 and spin-5/2 system consisting of two sublattices *A* and *B*, which are arranged alternately. The sublattice *A* are occupied by spins S_i^A, which takethe spin values of ± 5/2, ± 3/2, ± 1/2, while the sublattice *B*are occupied by spins S_j^B, which take the spin values of ± 3/2, ±1/2. In each site of the lattice, there is crystal-field constants,$D_A$in the sublattices *A* and $D_B$in the sublattice *B* acting on the spin-3/2 and spin-5/2 respectively. The Hamiltonian of the system according to the mean-field theory is given by

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

where the first summation is carried out only over nearest-neighbour pairs of spins on different sublattices and *J* is the nearest-neighbour exchange interaction. In order to treat the model approximately we employ a variational method based on the Bogoliubov inequality for the Free energy [20],

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

where $F(\mathcal{H})$ is the true free energy of the model described by Hamiltonian given in (1). $F_0(\mathcal{H})$is the model described by the trial Hamiltonian $\mathcal{H}_0$which depends on variational parameters, and $\langle\cdots\rangle_0$ denotes a thermal average over the ensemble defined by $\mathcal{H}_0$. Now, depending on the choice of the trial Hamiltonian, one can construct approximate methods of different accuracy. However, owing to the complexity of the problem, we consider in this work the simple choice of $\mathcal{H}_0$, namely,

$$\mathcal{H}_0 = -\sum_i\left(\gamma_A S_i^A + D_A\left(S_i^A\right)^2\right) - \sum_j\left(\gamma_B S_j^B + D_B\left(S_j^B\right)^2\right) \qquad (3)$$

where A and B are the two variational parameters related to 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. The approximated free energy is then obtained by minimizing the right hand side of Eq. (2) with respect to variational parameters.

Because of the simplicity of $\mathcal{H}_0$, it is easy to evaluate the expressions in (3) and substitute in (2) to obtain

$$f \equiv \frac{\emptyset}{N} \leq \frac{-1}{2\beta}\left[\begin{array}{l} \ln\left[\begin{array}{c} \exp\left(\frac{25}{4}\beta D_A\right)\left(2\cosh\frac{5}{2}\beta\gamma_A + \exp(-4\beta D_A)\right. \\ \left(2\cosh\frac{3}{2}\beta\gamma_A\right) + \exp(-6\beta D_A)\left(2\cosh\frac{1}{2}\beta\gamma_A\right)\Big) \end{array}\right] \\ + \ln\left[\exp\left(\frac{9}{4}\beta D_B\right)\left(\begin{array}{c} 2\cosh\frac{3}{2}\beta\gamma_B + \exp(-2\beta D_B) \\ \left(2\cosh\frac{1}{2}\beta\gamma_B\right) \end{array}\right)\right] \end{array}\right]$$

$$+\frac{1}{2}\left[-z\,\langle S_i^A\rangle_0\langle S_j^B\rangle_0 + (\gamma_A - H)\langle S_i^A\rangle_0 + (\gamma_B - H)\langle S_j^B\rangle_0\right] \quad (4)$$

Where $\beta = -\frac{1}{k_B T}$, N is the total number of sites of the lattice and z is its coordination number. The sublattice magnetizations per site m_A; m_B are denoted by

$$m_A = \langle S_i^A\rangle$$

$$= \frac{\frac{5}{2}\mathrm{s}\left(\frac{5}{2}\beta\gamma_A\right)+\frac{3}{2}e^{-4D_A\beta}\,\mathrm{s}\left(\frac{3}{2}\beta\gamma_A\right)+\frac{1}{2}e^{-6D_A\beta}\,\mathrm{s}\left(\frac{1}{2}\beta\gamma_A\right)}{\mathrm{c}\left(\frac{5}{2}\beta\gamma_A\right)+e^{-4D_A\beta}\,\mathrm{c}\left(\frac{3}{2}\beta\gamma_A\right)+e^{-6D_A\beta}\,\mathrm{c}\left(\frac{1}{2}\beta\gamma_A\right)} \quad (5)$$

$$m_B = \langle S_j^B\rangle = \frac{\frac{3}{2}\mathrm{s}\left(\frac{3}{2}\beta\gamma_B\right)+\frac{1}{2}e^{(-2D_B\beta)}\,\mathrm{s}\left(\frac{1}{2}\beta\gamma_B\right)}{\mathrm{c}\left(\frac{3}{2}\beta\gamma_B\right)+e^{(-2D_B\beta)}\,\mathrm{c}\left(\frac{1}{2}\beta\gamma_B\right)} \quad (6)$$

To evaluate the phase diagram (second-order phase transition lines) of a mixed-spin system, one has to expand Eqs.((4),(5),(6)), that :

$f = f_0 + am_A^2 + bm_A^4 + m_A^6 + \cdots$ (7)

where the coefficients f_0 and a are given by :

$$f_0 = -\frac{1}{2\beta}\ln\Big[\exp\Big(\frac{25}{4}d\ \Big)(2 + 2\exp(-4d\ )$$

$$+2\exp(-6d\ )\big) + \exp\Big(\frac{9}{4}d\ \Big)(2 + 2\exp(-2d\ ))\Big], \qquad (8)$$

and

$$a = \Big(6.25\frac{B(2.25B + 0.25\,Be^{-2d}\ )}{1.0 + e^{-2d}} + \frac{2.25Be^{-4d}\ (2.25B + 0.25Be^{-2d}\ )}{1.0 + e^{-2d}} + \frac{0.25Be^{-6d}\ (2.25B + 0.25Be^{-2d}\ )}{1.0 + e^{-2d}}\Big) / (1.0 + e^{-4B} + e^{-6B}\ ).$$

Where, $b = \beta$, $d = \beta D_A$, $d = \beta D_B$.

In this way, critical points are determined as second-order transition lines when *a=0*. Further, it should be noted that the coefficient *a* is even function of *J*. Therefore, the critical behavior is the same for both ferromagnetic (*J >0*) and ferrimagnetic (*J <0*) systems. On the other hand, in the ferrimagnetic case the signs of the sublattice magnetizations are different, and there may be a compensation temperature T_k ($T_k<T_c$) at which the total magnetization per site

$M = \frac{m_A+m_B}{2.0}$(8)

is equal to zero, although $m_A \neq 0$. and $m_B \neq 0$. In particular, to prove whether the present mixed-spin system can exhibit a compensation points or not, we shall consider below *J < 0*.

3. RESULTS AND DISCUSSIONS

3.1 Ground State Phase Diagram

We begin with the ground-state structure of the system. At zero temperature, The ground-state phase diagram is easily determined from Hamiltonian (1) by comparing the ground-state energies of the different phases, and is shown in Fig. 1. At zero temperature, we find six ordered phases with different values of {m_A, m_B, q_A, q_B }, namely the ordered ferrimagnetic phases. These ordered phases are separated by first ordered lines and the values{m_A, m_B, q_A, q_B } for these phases are given as following:

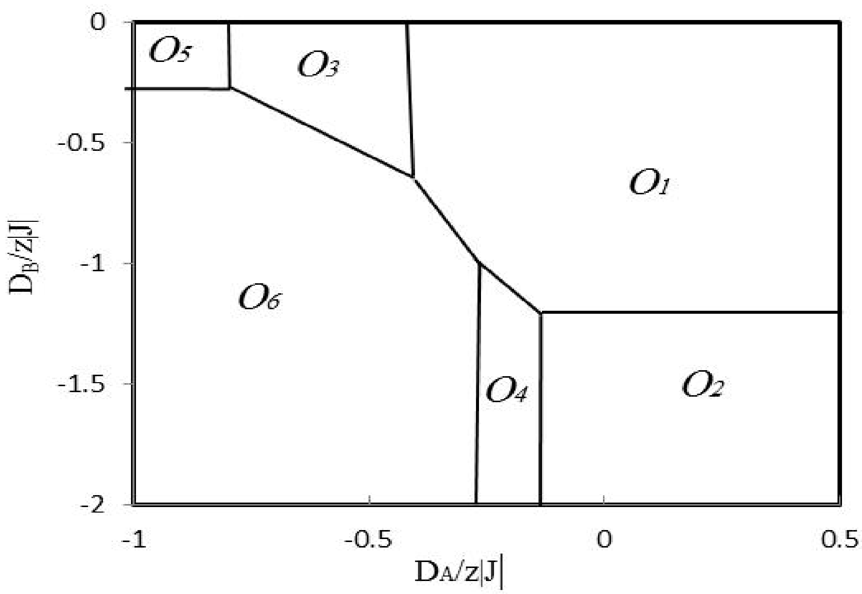

Fig. 1 Ground-state phase diagram of the mixed spin-3/2 and spin-5/2 Ising ferrimagnetic system with the coordination number *z* and different crystal-field constants D_A *z* |*J* |and D_B/ *z* |*J*| The four ordered phases are O_1 ,O_2, O_3, O_4, O_5, O_6 , and there are no disordered phases in the ground-state phase diagram

3.2 Compensation Temperature

A compensation temperature T_k of the system can be evaluated by requiring the condition M = 0 in the coupled Eqs. (5) and (6).

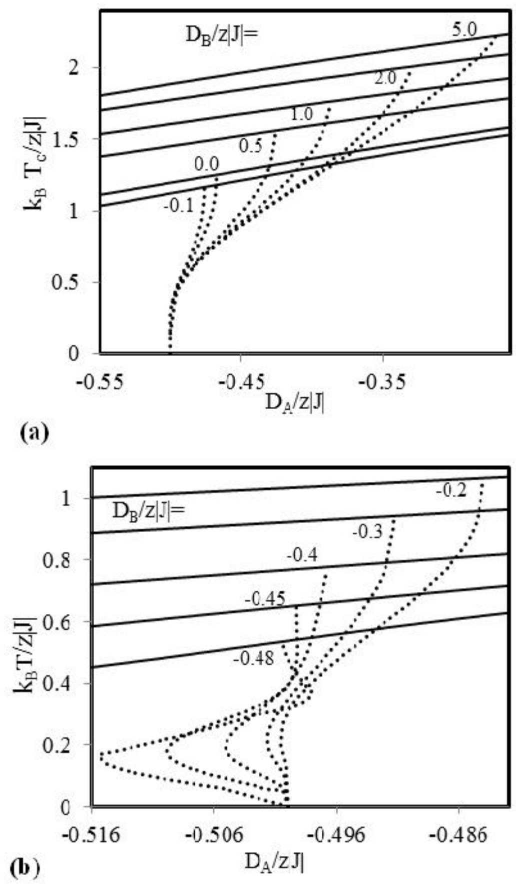

Fig. 2 Dependence of the compensation temperature (dotted curves) on crystal-field constant*DA*/*z*|*J*| in a mixed-spin Ising ferrimagnet with the coordination number *z*, when the value of *DB*/*z*|*J*| is changed. (a) The curves show the positions of one and two compensation points only; (b) The curves show the positions of one, two and three compensation points. The solid curves represent the second-order transitions.

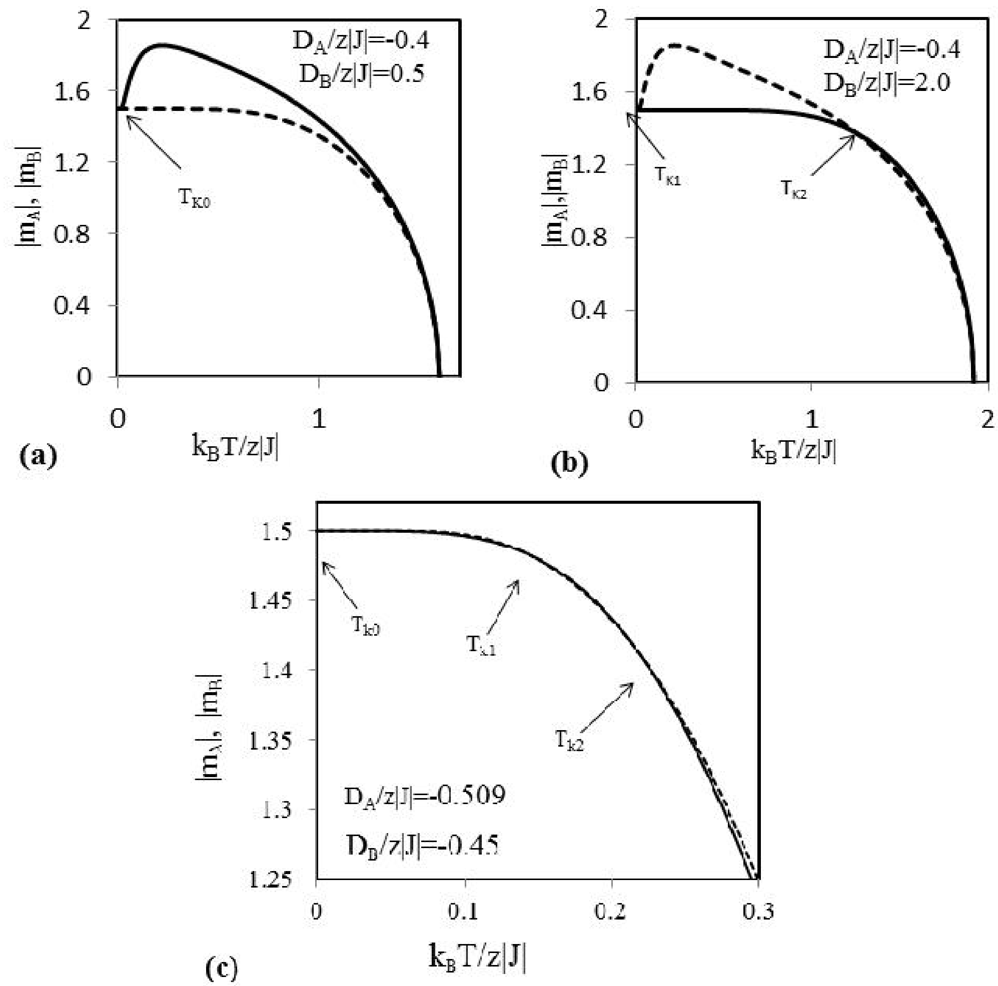

Fig. 3. The thermal dependences of the sublattice magnetizations $|m_A|$ (solid line) and $|m_B|$ (dashed line) for the mixed-spin Ising ferrimagnet with coordination number z, when $D_A/z|J| = -0.4$ and $D_B/z|J| = 0.5$ in (a), $D_A/z|J| = -0.4$ and $D_B/z|J| = 2.0$ in (b) and $D_A/z|J| = -0.509$ and $D_B/z|J| = -0.45$ in (c).

Now, let us investigate whether the present mixed-spin Ising ferrimagnetic system may exhibit a compensation point (or points) at $T \geq 0$ when the single-ion anisotropies are changed.

The variation of the compensation temperature T_k as function of $D_A/z|J|$ is shown in Fig. 2 for several values of $D_B/z|J|$. As seen from the figure 2 (a), for the selected values of D_B = -0.1, -0.0, 0.5, 1.0, 2.0, 5.0, all the T_k curves emerge from $D_A/z|J|$ = -0.5 at T = 0K and increase monotonically with $D_A/z|J$; to terminate at the corresponding phase boundaries (solid lines) which implies the occurrence of one compensation point in the system. As $D_B/z|J|$ is reduced, the range of $D_A/z|J|$ over which the compensation point occurs gradually becomes small, but the compensation temperature still reaches the corresponding transition line

In fig.2 (b), we can see a new type of compensation temperature curves in a restricted region of $D_A/z|J$, when $D_A/z|J< -0.5$ and $D_B/z|J|$ takes the selected values -0.2, -0.3, -0.4,.-0.45 and -0.48. In this case, the compensation temperature lines exhibit bulges, which implies the occurrence of two compensation points in the system.

Typical sublattice magnetization curves with a compensation point at T = 0K; T≠ 0K and with two and three compensation points are shown in Figs. 3 (a)–(c), respectively. Note that the existence of the compensation temperature at T =0 K corresponds to the ordered phase O_3 where $S_i^A = \frac{3}{2}$ and $S_j^B = -\frac{3}{2}$, for all the three cases in fig. 3. See (fig 1), the ground state phase diagram.

In fig.3.(a), for $D_A/z|J| = -0.4$ and $D_B/z|J| = 0.5$, sublattice magnetizations $|m_A|$and$|m_B|$take the saturation values $|m_A|=|m_B|=\frac{3}{2}$ with one compensation point at T = 0K, in agreement with the ground-state phase diagram, and there are no compensation points for all the values of T>0K.In fig.3.(b), for $D_A/z|J| = -0.4$ and $D_B/z|J| = 2.0$, sublattice magnetizations $|m_A|$and$|m_B|$ have

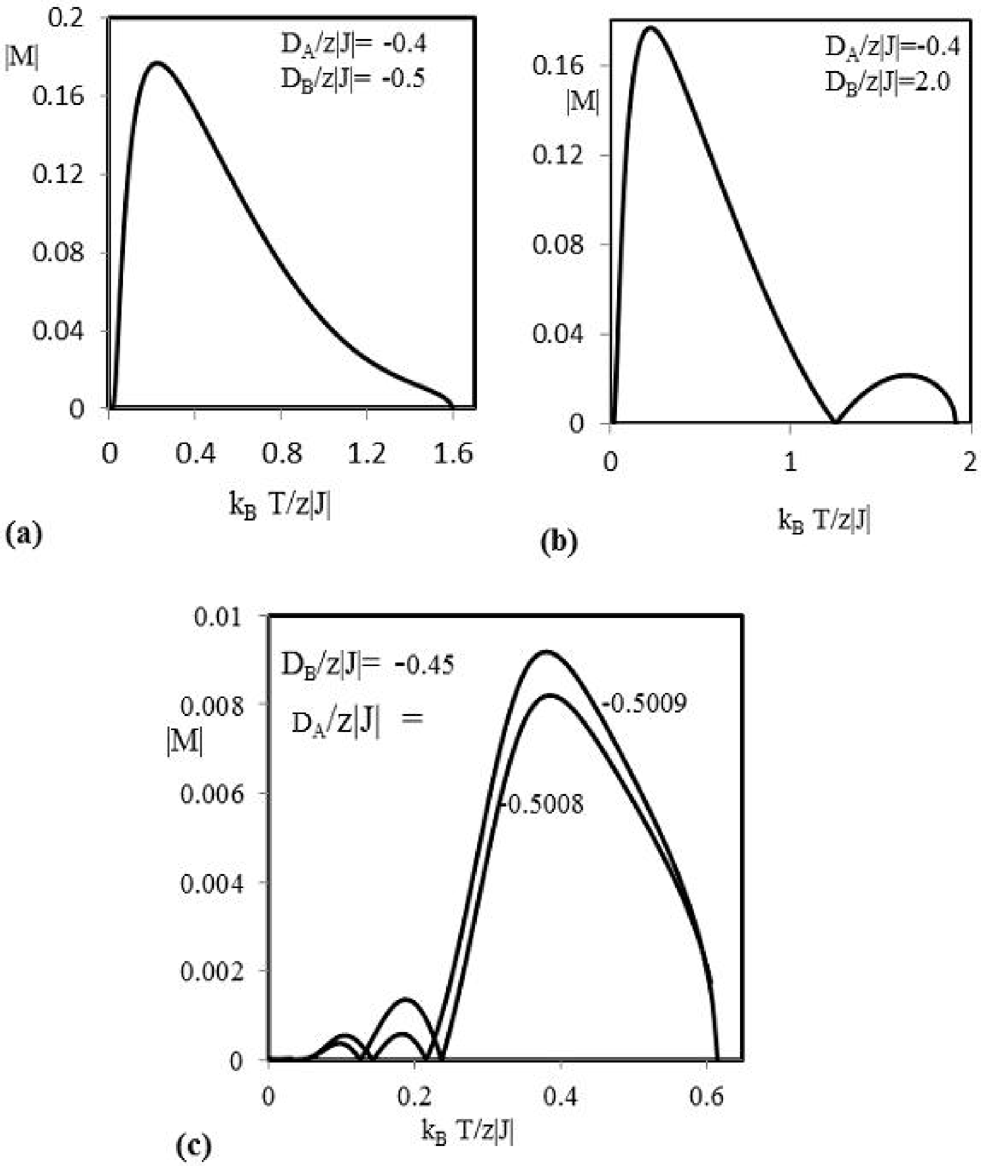

Fig. 4. Thermal variations of the total magnetization |M| for the mixed-spin Ising ferrimagnet with the coordination number z, when the value of $D_B/z|J|$= 0.5, $D_A/z|J|$ = −0.4 in (a), $D_B/z|J|$= 2.0, $D_A/z|J|$ = −0.4 in (b) and $D_B/z|J|$= -0.45, $D_A/z|J|$ = −0.4008 and -0.4009 in (c).

the saturation values $|m_A|= |m_B| = \frac{3}{2}$ at T = 0K, causing one compensation point T_{K0} at T=0 K. As the temperature increased, the sublattice magnetization $|m_A|$ exhibits a rapid increase at $T \to 0K$ before it decreases from its highest value to compensate at the compensation temperature T_{K1} with the sublattice magnetization $|m_B|$ which displays a standard characteristic convex shape.

In this case, it is clear from fig 3.(b) that the system exhibits two compensation points T_{K0} and T_{K1}. Finally, as shown in fig 3(c) the magnetization $|m_A|$ may be reduced below that of B-sublattice, before the sublattice magnetizations fall to zero at the critical point. As a result, an additional compensation point T_{K3} may appear at a high temperature in the system. In this case, the system exhibits three compensation points withappropriate negative values of $D_A/z|J$ and $D_B/z|J$. ($D_A/z|J| =-0.509$ and $D_B/z|J|= -0.45$.

Typical sublattice magnetization curves (|M| versus k_B T/z|J|) which refer to the compensation temperatures presented in fig. 3(a), (b) and (c) are shown in Fig. 4 (a), (b) and (c) respectively. In these three figures, we can see one compensation point at zero temperature in fig 4(a), two compensation points in fig 4(b) and three compensation points in fig 4(c). These results can be compared with the results presented in previous papers as [23-25]

In particular, in fig.4 (b) (the case of two compensation points), one can observe that the magnitude of the total magnetization between the compensation point and transition temperature is always smaller than that between the two compensation points, but in fig. 4(c) (the case of three compensation points) the magnitude of the total magnetization between the two compensation points is always smaller than that between the compensation point and transition temperature.

4. CONCLUSIONS

In this work, we have studied the effect of the crystal-field constants on the compensation temperatures of a mixed-spin Ising system consisting of spin-5/2 and spin-3/2 with different crystal-field constants D_A and D_B acting on the spin-5/2 and spin-3/2, respectively. In this consideration, we have applied the mean-field theory based on Bogoliubov inequality for the Gibbs free energy. The compensation temperature lines versus the crystal-field constant D_A at selected values of crystal-field constant D_B are shown. We observed that these curves emerge from $D_A/z|J| = -0.5$ at T= 0K and increase with $D_A/z|J$; to terminate at the corresponding phase boundaries. We also observed that this mixed-spin ferrimagnetic system may exhibit one, two or three compensation points. These results can be compared with the results appeared in the literature [21], [22], [23]. We believe that 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 researchon such materials, and we wish that this work could simulate further theoretical and experimental works on ferrimagnetic materials.

REFERENCES

[1] O. Khan, Molecular Magnetism, VCH Publishers, NewYork, 1993.
[2] T. Mallah, S. Thiebaut, M. Vardegauer, P. Veillet, Science 262 (1993) 1554.
[3] H. Okawa, N. Matsumoto, H. Tamaki, M. Ohba, Mol. Cryst. Liq. Cryst. 233 (1993) 257.
[4] C. Mathoniere, C.J. Nutall, S.G. Carling, P. Day, Inorg. Chem. 35 (1996) 1201.
[5] Y. Nakamura, Phys. Rev. B 62 (17) (2000) 11742.
[6] Y. Belmamoun, M. Kerouad, Chinese J. Phys. 47 (1) (2009) 100.
[7] A. Benyoussef, A. ElKenz, M. Elyadari, M. J. Cond. Matter 8 (1) (2007) 72.

[8] G.M. Buendia, J.A. Liendo, J. Phys.: Condens. Matter 9 (1997) 5439.
[9] L. Neel, Ann. Phys. Paris 3 (1948) 137.
[10] A.E. Berkowitz, K. Takano, J. Magn. Magn. Mater. 200 (1999) 552.
[11] A. Bobak, M. Jurcisin, Physica B 233 (1997) 187.
[12] A. Bobak, Physica A 258 (1998) 140.
[13] Z.H. Xin, G.Z. Wei, T.S. Liu, J. Magn. Magn. Mater. 188 (1998) 65.
[14] G.Z. Wei, Z.H. Xin, J. Wei, J. Magn. Magn. Mater. 204 (1999) 144.
[15] A. Bobak, Physica A 286 (2000) 531.
[16] A. Bobak, O.F. Abubrig, D. Horvath, J. Magn. Magn. Mater. 246 (2002) 177.
[17] J.W. Tucker, J. Magn. Magn. Mater. 237 (2001) 215.
[18] O.F. Abubrig, D. Horvath, A. Bobak, M. Jascur, Physica A . 296 (2001) 437.
[19] E. Albayrak, Phys. Status Solidi B 239 (2003) 411.
[20] E. Albayrak, Int. J. Mod. Phys. B 17 (2003) 1087.
[21] F. Abubrig, Open J. of Applied Sciences. 3 (2013) 218-223. [22] F. Abubrig, Open J. of Applied
[22] F. Abubrig, Open J. Applied Sciences. 3 (2013) 270-277.
[23] E. Albayrak, Physica B 391 (2007) 47–53.
[24] E. Albayrak, Physica A. 375 (2007) 174-184.
[25] B. Deviren, E. Kantar, M. Keskin, J. Magn. Magn. Mater. 56 (2010) 1738-1747.
[26] M. Karimou1, R. Yessoufou, F. Hontinfinde,World J of Condensed Matter Physics. 5 (2015) 187-200.
[27] Hadey K. Mohamad, International Letters of Chemistry, Physics and Astronomy57 (2015) 114-121.
[28] N. De La Espriella Velez, J. Madera Yancez, M. S. Paez Mesa, Revista Mexicana de Fısica 60 (2014) 419–424.
[29]A. Jabar, R. Masrour,A. Benyoussef, M. Hamedoun, J. Magn. Magn. Mater. 397 (2016) 287-294.