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RESEARCH ARTICLE

Spin Compensation Temperatures in the Mean-field Theory of a Mixed Spin-3/2 and Spin-7/2 Blume-Capel Ising Model

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Abstract

In this research it has been constructed the ground-state phase diagram of a mixed spin-3/2 and spin-7/2 Blume-Capel Ising system on a square lattice in the (D_A, D_B) plane. Magnetic phase transitions, in a molecular based magnet, are tested using mean field method (MFM). The equilibrium magnetizations can be achieved by minimizing the free energy which is vital for locating and spin compensation points as well. By utilizing mean field theory (MFT) on principles of Bogoliubov inequality of the free energy, it has been investigated the spin compensation phenomena. In particular, characteristic ferrimagnetic features have been shown depending on the negative values of the different single-ion anisotropies D_A, D_B, acting on the $A-$atoms and $B-$atoms, respectively.

Keywords: *Blume-Capel Ising model; Ground-state phase diagram; Compensation temperature; Magnetic free energy.*

Introduction

Recently, many researchers experimentally worked in the area of molecular based magnetic materials. These materials are compounds play an important role on supporting the storage applications and the density speed [1]. The heterocomplex, in particular

$[Cr(CN)_4(\mu-CN)_2Gd(H_2O)_4-(bpy)]_n.4nH_2O.1.5nbpy$,

has been synthesized successfully. It contains the gadolinium $Gd(III)$ and chromium $Cr(III)$ atoms which are coupled ferrimagetically. The magnetization variations under the effects of both temperature and the presence of magnetic fields of the gadolinium orthochromate $GdCrO_3$, where the Cr^{3+} and Gd^{3+} moments possess anti-parallel coupling may have been discovered [2].Theoretical investigations, in this respect, are intensively studied as simple models that can be shown ferrimagnetic behaviors. It is worthy note that the ground-state phase diagrams are useful to reveal regions that important magnetic behaviors could arise [3, 9]. J.S. da Cruz Filho et al constructed the ground-state phase diagram of the spin-2 and spin-5/2 mixed Ising Model at absolute zero temperature in the anisotropy space [10].So, the researchers inspected the presence and dependence of compensation points on single-ion anisotropies. They examined the influence of different crystal fields on the critical temperature of the mixed Ising ferrimagnets, in the light of reliability of the numerical results for the phase diagrams at finite temperature [11, 13].

One has found that the compensation temperatures increase with increasing the values of both single-ion anisotropies. On the other hand, N. De La Espriella et al [14] investigated the behavior of ground state phase diagrams of a mixed Ising system on a bipartite square lattice and proposed that the Hamiltonian includes coupling to first and second neighbors, respectively. In this correspondence, it has been studied a Blume-Capel Ising ferrimagnetic system with mixed spin on a square lattice in which the two mixing sublattices have spins $(\pm 1/2, \pm 3/2)$ and spins $(\pm 1/2, \pm 3/2, \pm 5/2, \pm 7/2)$. First, it has been constructed the ground-state phase diagram of the proposed system in the $(D_A/|J|, D_B/|J|)$ plane. Within the mean field approximation based on the Bogoliubov inequality for the free energy, it has been surveyed the spin compensation phenomena of the model. So, distinctive ferrimagnetic behaviors have been attained based on, exclusively, the negative values of the magnetic anisotropies D_A, D_B, acting on the $A-$atoms and $B-$atoms, respectively.

Theory

In this paper the system which is considered consists of two interpenetrating sublattices. One sublattice has spins (σ_i^A) take four values, and the other sublattice has spins (σ_j^B) taking eight values. So, the Hamiltonian of the mixed spin Blume–Capel Ising ferrimagnetic system is given as [7, 10]:

$$H = -J\sum_{i,j}\sigma_i^A\sigma_j^B - D_A\sum_i(\sigma_i^A)^2 - D_B\sum_j(\sigma_j^B)^2 \tag{1}$$

Where the sites of sublattice A are occupied by spins σ_i^A taking the values of ± 1/2, ± 3/2, and the sites of sublattice B occupied by spins σ_j^B can take the values of ± 1/2, ± 3/2, ± 5/2, ± 7/2. D_A, D_B Are the anisotropies affecting on A-sites and B-sites, respectively. J Is the exchange interaction parameter (J <0).By manipulating the Hamiltonian through using Bogoliubov Inequality, the free energy of the model is estimated [7, 10], such that:

$$F \le F_0 + \langle H - H_0\rangle_0 \tag{2}$$

Where F is the free energy of H given by (1), and,

$$H_o = -\sum_i[\lambda_A\sigma_i^A + D_A(\sigma_i^A)^2] - \sum_j[\lambda_B\sigma_j^B + D_B(\sigma_j^B)^2] \tag{3}$$

Minimizing the right hand of Eq. (2) with respect to variational parameters, one can obtain the approximated free energy as,

$$\begin{aligned} F \equiv \frac{\Phi}{N} = -\frac{1}{2\beta}\{&\ln[2e^{9/4\beta D_A}\cosh(\frac{3}{2}\beta\lambda_A) + 2e^{1/4\beta D_A}\cosh(\frac{1}{2}\beta\lambda_A)] + \\ &\ln[2e^{49/4\beta D_B}\cosh(\frac{7}{2}\beta\lambda_B) + 2e^{25/4\beta D_B}\cosh(\frac{5}{2}\beta\lambda_B) + 2e^{9/4\beta D_B}\cosh(\frac{3}{2}\beta\lambda_B) + 2e^{1/4\beta D_B}\cosh(\frac{1}{2}\beta\lambda_B)]\} + \\ &1/2(-zJm_Am_B + \lambda_Am_A + \lambda_Bm_B) \end{aligned} \tag{4}$$

Where N is the total number of sites of lattice? Minimizing this expression with respect to λ_A, λ_B, that one has,

$$\lambda_A = Jzm_B\ ,\ \lambda_B = Jzm_A, \tag{5}$$

With,

$$m_A \equiv \langle\sigma_i^A\rangle_o = \frac{1}{2}\frac{3\sinh(1.5\beta\lambda_A) + e^{-2\beta D_A}\sinh(0.5\beta\lambda_A)}{\cosh(1.5\beta\lambda_A) + e^{-2\beta D_A}\cosh(0.5\beta\lambda_A)} \tag{6}$$

$$m_B \equiv \langle\sigma_j^B\rangle_o = \frac{1}{2}\frac{7\sinh(3.5\beta\lambda_B) + 5e^{-6\beta D_B}\sinh(2.5\beta\lambda_B) + 3e^{-10\beta D_B}\sinh(1.5\beta\lambda_B) + e^{-12\beta D_B}\sinh(0.5\beta\lambda_B)}{\cosh(3.5\beta\lambda_B) + e^{-6\beta D_B}\cosh(2.5\beta\lambda_B) + e^{-10\beta D_B}\cosh(1.5\beta\lambda_B) + e^{-12\beta D_B}\cosh(0.5\beta\lambda_B)} \tag{7}$$

Where $\beta = \frac{1}{K_BT}$, z is the number of nearest neighbor sites?

The signs of sub lattice magnetizations are opposite in the ferrimagnetic region, hence there may be a spin compensation temperature were the interpenetrating sublattice magnetizations annihilated [7, 15].

Results and Discussions

The mixed spin-3/2 and spin-7/2 Blume-Capel Ising Models expose eight phases with various values of $\{m_A, m_B, R_A, R_B\}$, i.e., the ordered ferromagnetic phases:

$$O_1 \equiv \{-\frac{3}{2},\frac{7}{2},\frac{9}{4},\frac{49}{4}\}, or\{\frac{3}{2},-\frac{7}{2},\frac{9}{4},\frac{49}{4}\}; O_2 \equiv \{-\frac{1}{2},\frac{7}{2},\frac{1}{4},\frac{49}{4}\}, or\{\frac{1}{2},-\frac{7}{2},\frac{1}{4},\frac{49}{4}\};$$
$$O_3 \equiv \{-\frac{3}{2},\frac{5}{2},\frac{9}{4},\frac{25}{4}\}, or\{\frac{3}{2},-\frac{5}{2},\frac{9}{4},\frac{25}{4}\}; O_4 \equiv \{-\frac{1}{2},\frac{5}{2},\frac{1}{4},\frac{25}{4}\}, or\{\frac{1}{2},-\frac{5}{2},\frac{1}{4},\frac{25}{4}\};$$
$$O_5 \equiv \{-\frac{3}{2},\frac{3}{2},\frac{9}{4},\frac{9}{4}\}, or\{\frac{3}{2},-\frac{3}{2},\frac{9}{4},\frac{9}{4}\}; O_6 \equiv \{-\frac{1}{2},\frac{3}{2},\frac{1}{4},\frac{9}{4}\}, or\{\frac{1}{2},-\frac{3}{2},\frac{1}{4},\frac{9}{4}\};$$
$$O_7 \equiv \{-\frac{3}{2},\frac{1}{2},\frac{9}{4},\frac{1}{4}\}, or\{\frac{3}{2},-\frac{1}{2},\frac{9}{4},\frac{1}{4}\}; O_8 \equiv \{-\frac{1}{2},\frac{1}{2},\frac{1}{4},\frac{1}{4}\}, or\{\frac{1}{2},-\frac{1}{2},\frac{1}{4},\frac{1}{4}\}$$

And the parameters R_A and R_B are defined as:

$$R_A = \left\langle (s_i^A)^2 \right\rangle, \qquad R_B = \left\langle (s_j^B)^2 \right\rangle \tag{8}$$

So, the corresponding ground-state energies per site for these phases are:

$$U_{O_1} = -\frac{21z|J|}{8} - \frac{9}{8}D_A - \frac{49}{8}D_B \tag{9}$$

$$U_{O_2} = -\frac{7z|J|}{8} - \frac{1}{8}D_A - \frac{49}{8}D_B \tag{10}$$

$$U_{O_3} = -\frac{15z|J|}{8} - \frac{9}{8}D_A - \frac{15}{8}D_B \tag{11}$$

$$U_{O_4} = -\frac{5z|J|}{8} - \frac{1}{8}D_A - \frac{25}{8}D_B \tag{12}$$

$$U_{O_5} = -\frac{9z|J|}{8} - \frac{9}{8}D_A - \frac{9}{8}D_B \tag{13}$$

$$U_{O_6} = -\frac{3z|J|}{8} - \frac{1}{8}D_A - \frac{9}{8}D_B \tag{14}$$

$$U_{O_7} = -\frac{3z|J|}{8} - \frac{9}{8}D_A - \frac{1}{8}D_B \tag{15}$$

$$U_{O_8} = -\frac{1z|J|}{8} - \frac{1}{8}D_A - \frac{1}{8}D_B \tag{16}$$

By comparing the energies (i.e., Eqs.(9)- (16)), one can create the ground-state phase diagram of the system with z=4, as shown in Fig.1.

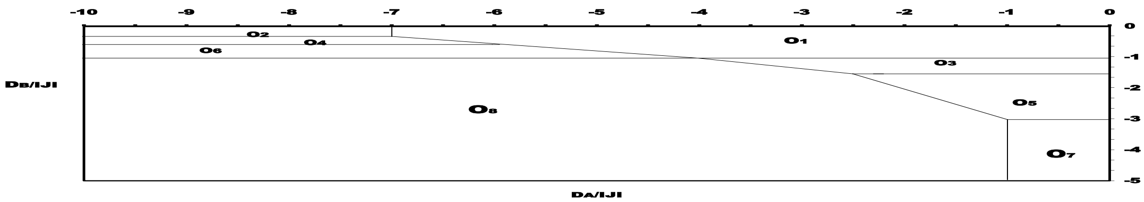


Fig.1: Ground state phase diagram of the considered model with the (z=4) nearest neighbors and different crystal fields D_A and D_B. The ordered phases: $O_1, O_2, O_3, O_4, O_5, O_6, O_7, O_8$,, are separated by thin lines, respectively

Now, let us consider the magnetic properties (i.e., spin compensation points and critical ones) of the mixed spin ferrimagnetic system with different crystal fields through which one can obtain characteristic magnetic behaviors of the system. Fig.2 resembles the global magnetization against the absolute temperature, in the absence of an external magnetic field, for different values of $D_A/|J|$.

It is interesting to examine the characteristic properties of the system that one can obtain a compensation temperature (T_k) for the $A-$ atoms and $B-$ ones when they are under the effect of particular values of crystal fields D_A, D_B, respectively. As shown in Fig.2, the system may exhibit characteristic features in the temperature dependence of the magnetization depending on the values of magnetic anisotropy D_A for a particular value of D_B, that it is possible to have two compensation points at $k_BT/|J|=0$ and $k_BT/|J|\neq 0$, respectively. It has been found that there is a response of the system for induction of two compensation temperatures in the range of negative values of anisotropy, namely, $-0.25 \leq D_A/|J| \leq -1.5$, with a fixed value of $D_B/|J|=-2.0$, of the sites occupied by B- atoms. One can observe Fig.(3), that the system does exhibit multicompensation points in the thermal variation of the system magnetization obtained by solving the coupled equations for m_A and m_B numerically.

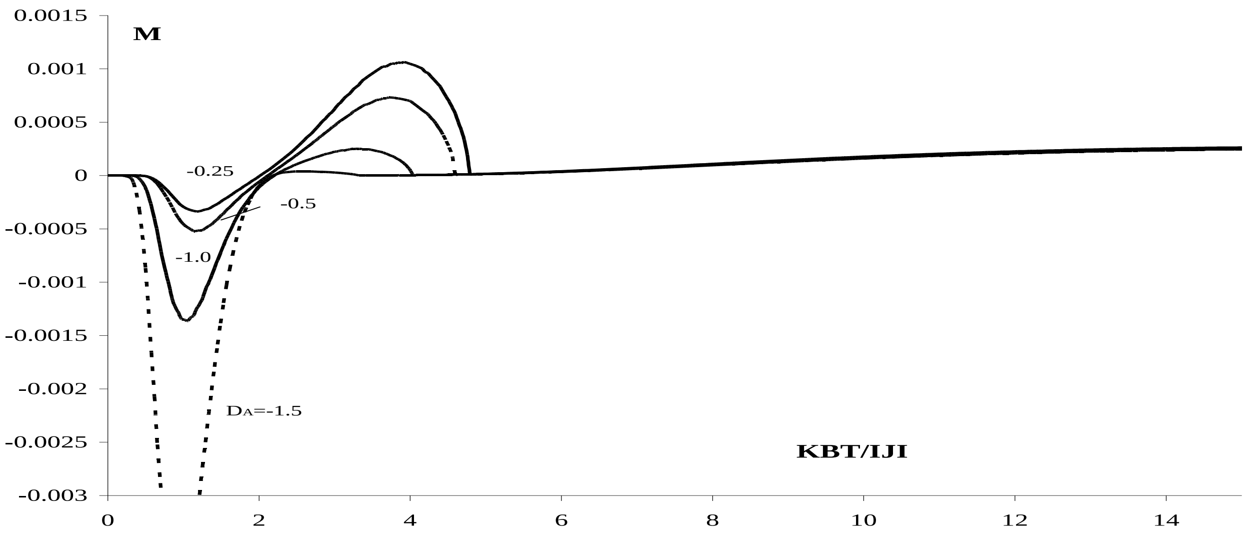


Fig.2: the global magnetization M versus temperature for the mixed–spin Ising ferrimagnet with z=4, when the value of $D_A/|J|$ is changed, for fixed $D_B/|J|=-2.0$

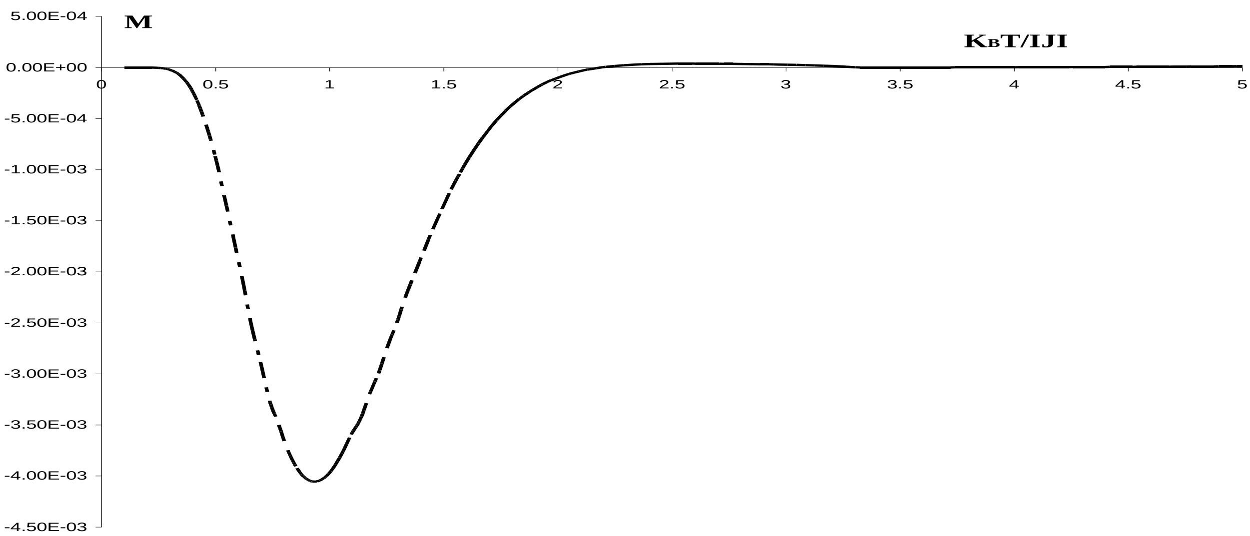


Fig.3. A close view the temperature variations of the magnetization for the mixed-spin Ising Ferrimagnet with z=4, when $D_B/|J|=-2.0$ and $D_A/|J|=-1.5$

At the points were the system may show two compensation temperatures, the magnetization of the interpenetrated sublattice m_A is more ordered than the magnetization of the interpenetrated sublattice m_B below the compensation point. These sublattice magnetizations are still incomplete so there is a residual magnetization in the system. As the values of $D_A/|J|$ are decreased, at particular values of crystal fields $D_B/|J|$ affecting on the B-atoms (one can observe Fig.3), the orientation of this remaining magnetization may change. However, due to entropy only a number of spins will flip their directions. Thus, the sublattice magnetization m_B turn out to be more ordered than the sublattice magnetization m_A for temperatures above the compensation point. At a point below the transition one will have a total cancellation of the global magnetization, i.e., a compensation temperature is happened [7, 12, 15].Now, let us discuss the temperature dependence of the sublattice magnetizations m_A and m_B by solving the coupled Eqs. (5)-(7) Numerically.

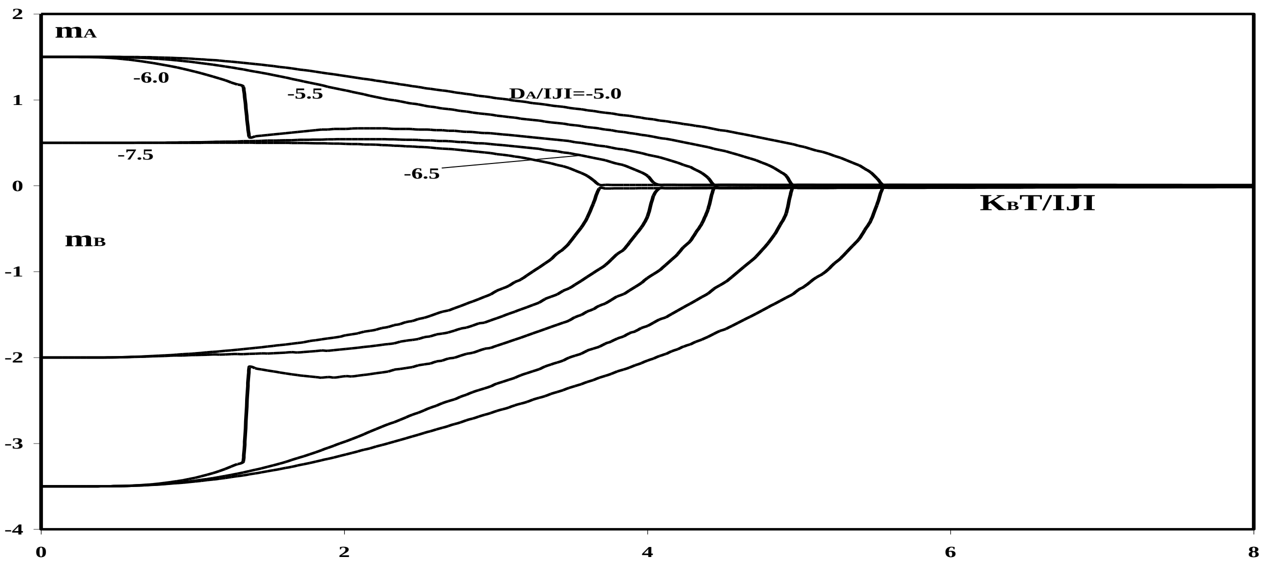


Fig.4: The temperature behavior of sublattice magnetizations m_A, m_B for the mixed–spin Ising ferrimagnet with z=4, for various values of $D_A/|J|$, and constant $D_B/|J| = -0.5$

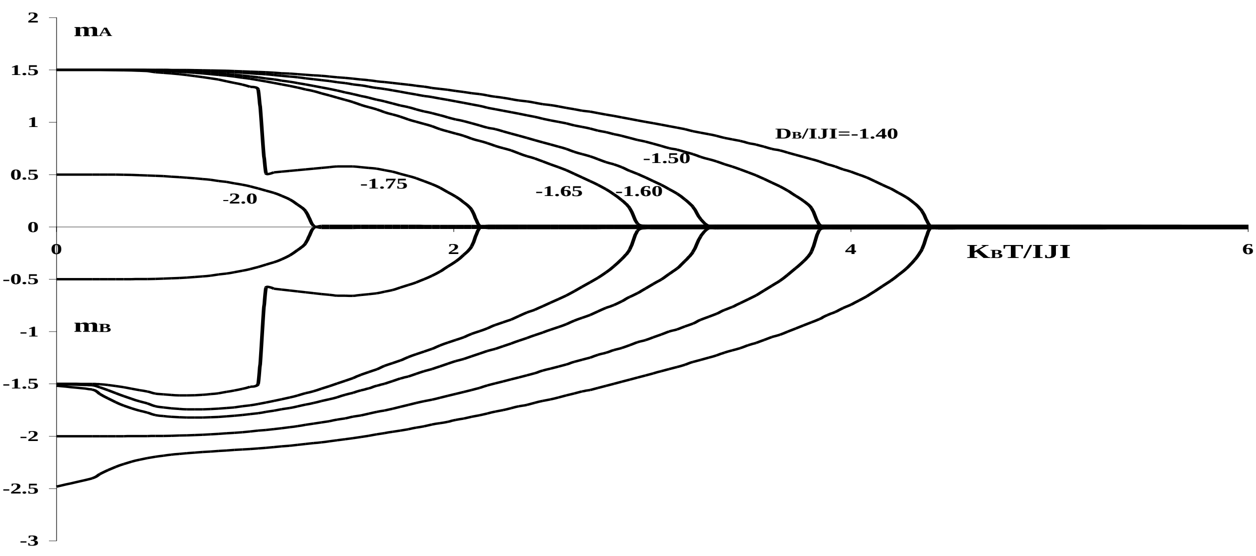


Fig.5: Thermal behavior of sub lattice magnetization m_A, m_B for the mixed–spin Ising ferrimagnet with the z=4, for several values of $D_B/|J|$, and constant $D_A/|J| = -2.25$

A case has been considered in the (m_A, T), (m_B, T) planes for the mixed-spin Ising ferrimagnet with coordination number z=4, when the values of $D_B/|J|$ and $D_A/|J|$ are changed, as shown in Figs.((4),(5)), respectively. In Fig.4, when $D_A/|J| \le -6.0$ for fixed $D_B/|J| = -0.5$, the sublattice magnetizations of mixture show a characteristic thermal variation behavior. So, the system shows that a sharp rapid increase from its saturation magnetization occurs. Within the range $D_A/|J| \ge -5.5$, the sublattice magnetization m_A shows a normal behavior (i.e., Q-type)[16]. Fig.5 refers to the thermal variations of the sublattice magnetizations m_A, m_B for the same system with the value of $D_B/|J|$ varies for a fixed value of $D_A/|J| = -2.25$.

For $-2.0 \le D_B/|J| \le -1.4$, the temperature dependence of m_A may exhibit a rather rapid decrease from its saturation value at $k_B T/|J| = 0$.The phenomenon is shown when the value of D_A approaches the critical value, in particular, at the critical value and for $T = 0K^o$, the saturation value of m_B is -2.0, indicating that in the ground state the spin configuration of the system consists of the mixed phase $s_j^B = \pm\frac{3}{2}$ or $s_j^B = \pm\frac{5}{2}$, with equal probability. One should notice that a new behavior, not predicted in the Ne'el theory of ferrimagnetism [15], observed in our model, when a value of $D_B/|J|$ approaches the critical one $D_{BC}/|J| = -1.5$. On the other hand, we have investigated the contribution of free energy to the thermodynamic phase stability of the mixed spin ferrimagnet which is considered. Free energy as a function of sublattices magnetizations has been calculated according to Eq.(4), is shown in Fig.6, and Fig. 7, respectively.

For the explanation of the free energy of the ferrimagnetic or antiferromagnetic state(at a compensation point $T < T_C$) and paramagnetic one(at transition temperature $T > T_C$), one can observe the free energy curve has an inflexion that it corresponds a discontinuous behavior and at a critical anisotropy value the free energy of the system is continuous, respectively.

So, the magnetization curves go to zero continuously separating the ferrimagnetic phase from the paramagnetic phase which is called the second-order phase transition or the Curie temperature. Whilst if a magnetization jump to either zero or to another value occurs there is the first-order phase transition temperature, or rather the temperature at which the magnetization jump occurs[6,7].The results shown in Figs. (6, 7) are consistent with those derived from Figs. (4, 5), respectively.

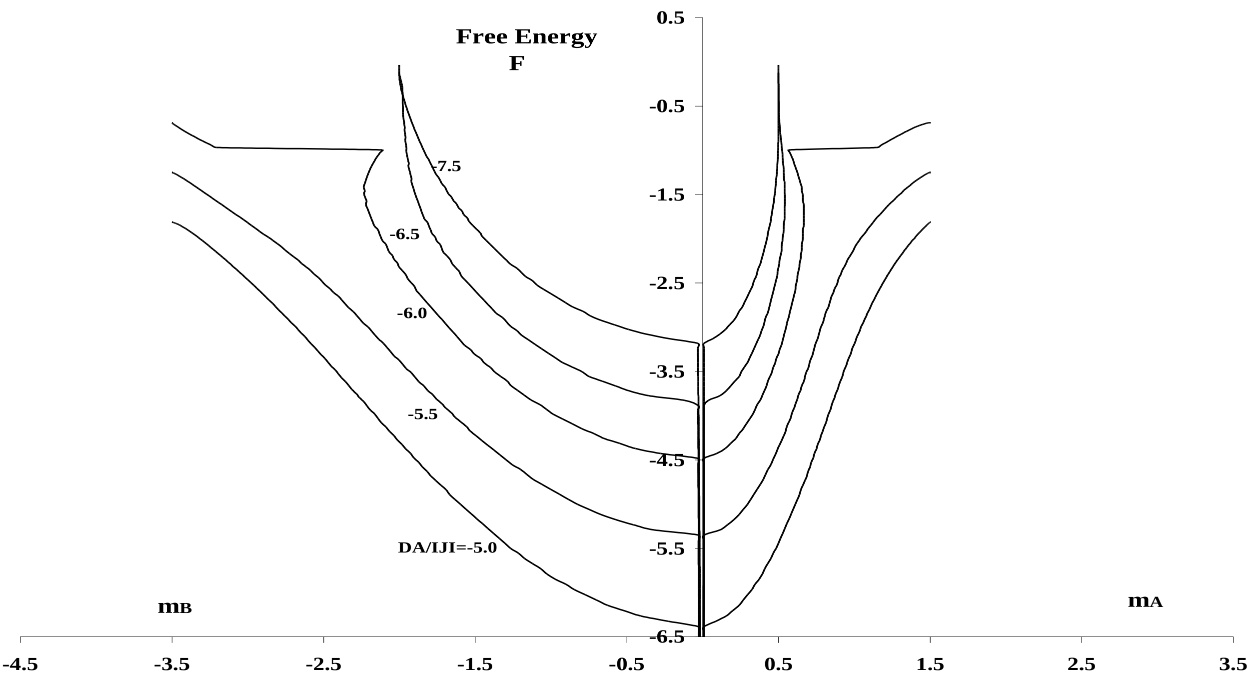


Fig.6: Free energy variations of the sublattices magnetizations for a square lattice of the mixed-spin ferrimagnet for different values of $D_A/|J|$, when the value of $D_B/|J| = -0.5$

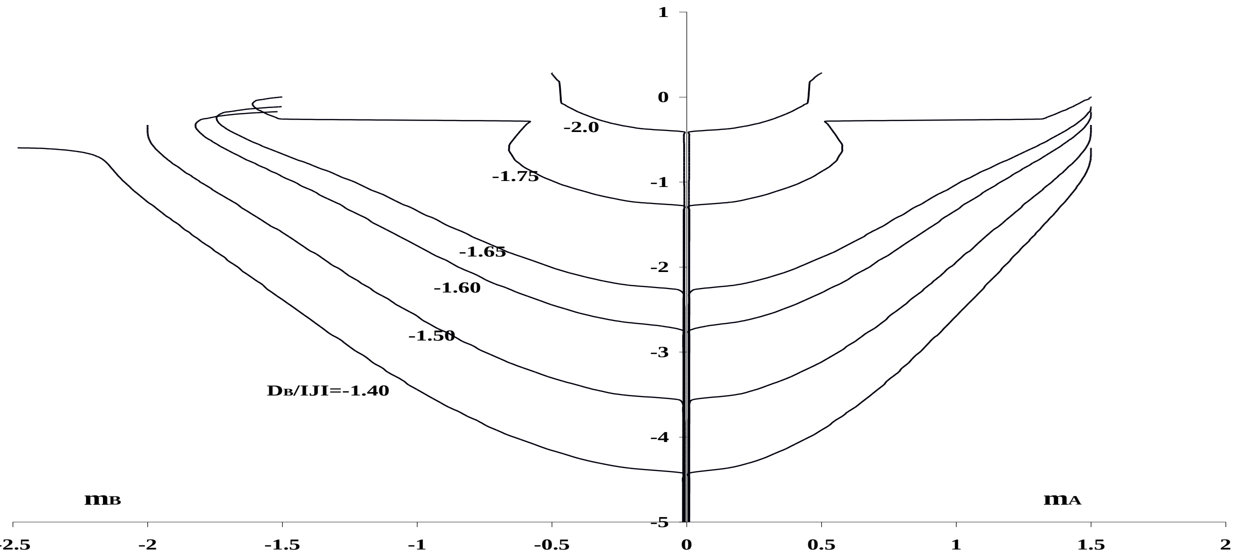
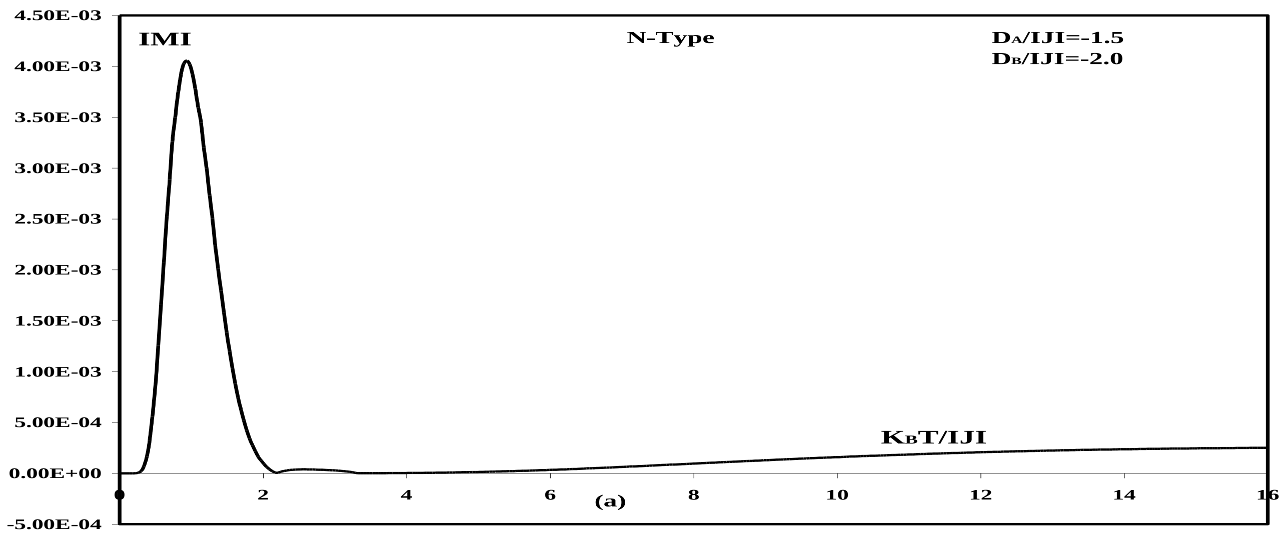
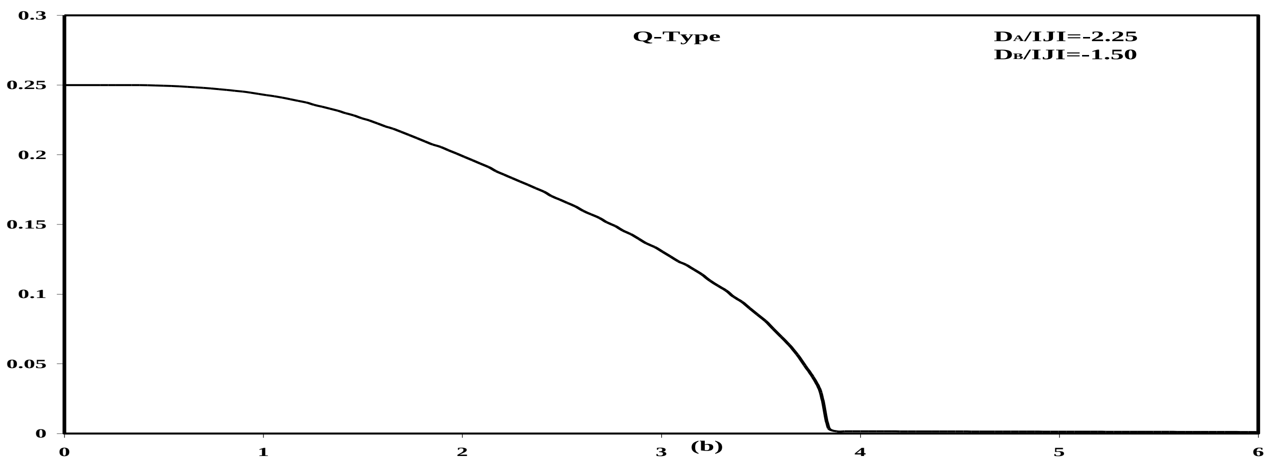


Fig.7: Free energy variations of the sublattices magnetizations for a square lattice of the mixed-spin ferrimagnet for different values of $D_B/|J|$**, when the value of** $D_A/|J| = -2.25$

Moreover, we have examined the total magnetization with thermal variations and acquired compensation types of the Blume-Capel Ising model. Fig.8 illustrates the thermal dependence of total magnetization |M| for certain values of anisotropies when z=4. One can observe Fig.8 that the considered model undergoes five types of different behaviors which are N-, Q-, R-, M-, and L-type, respectively. The appearance of these curves is strongly dependent on the crystal fields' values.





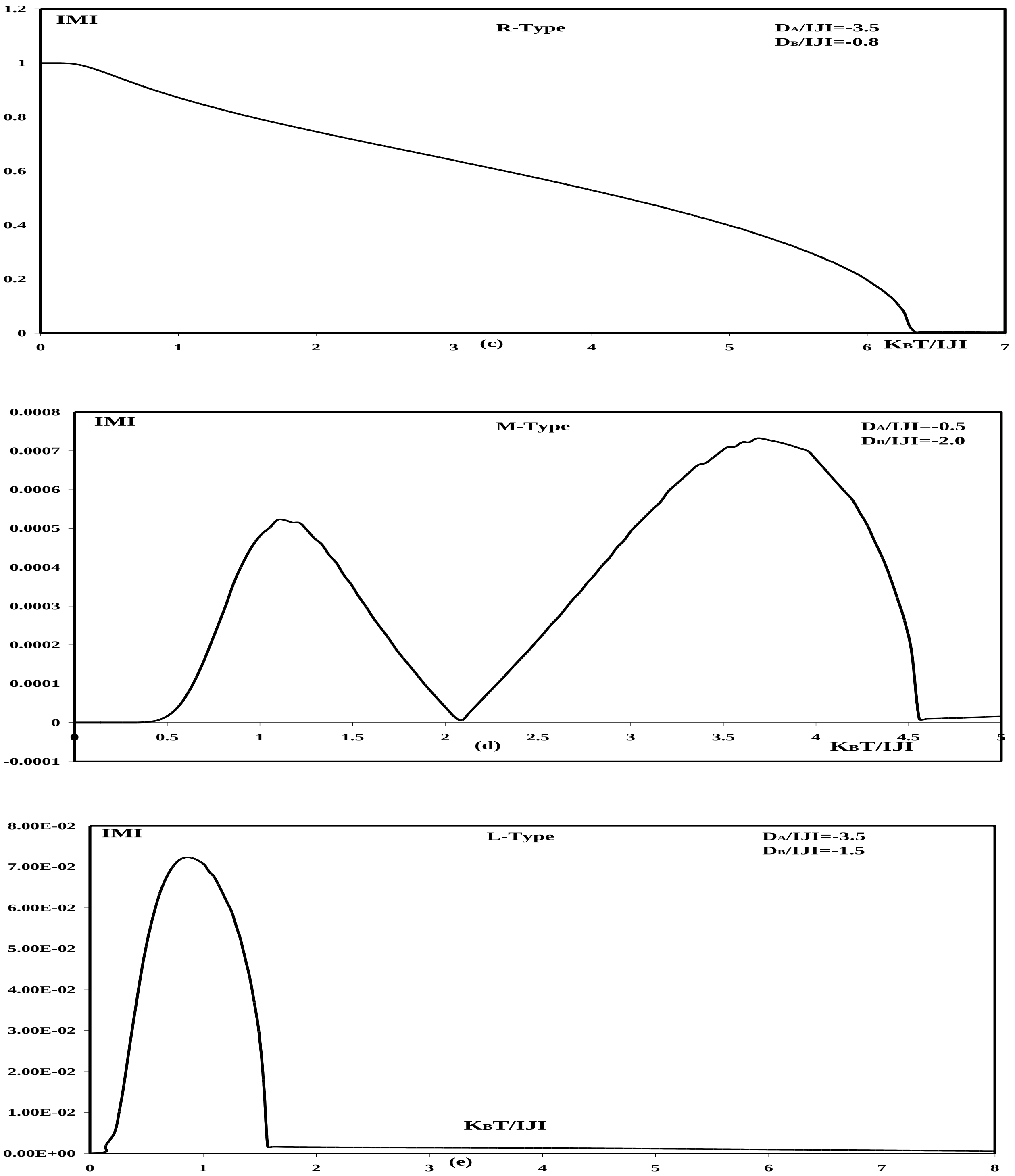


Fig.8: Different types of thermal dependence of magnetizations for z=4. (a) N-type for DA/|J|= -1.5, and DB/|J|= -2.0, (b) Q-type for DA/|J|= -2.25 and DB/|J|= -1.5 (c) R-type for DA/|J|= -3.5 and DB/|J|= -0.8 (d) M-type for DA/|J|= -0.5 and DB/|J|= -2.0, (e) L-type for DA/|J|= -3.5 and DB/|J|= -1.5

Conclusions

The phase diagram of the ground-state for the mixed spin-3/2 and spin-7/2 Ising ferrimagnet with Blume-Capel term included has been created. The magnetic assets of the system with different crystal fields have been found by solving the general expressions numerically. So, the magnetization curves have shown some outstanding features (two compensation temperatures). Thus, the obtained outcomes can be compared with those of a mixed spin-3/2 and spin-5/2 system[3], and the mixed spin-3/2 and spin-2 on the basis of Bethe lattice[5], showing one or two compensation temperatures based on the values of the crystal fields, respectively. Furthermore, a theoretical study for a mixed spin-5/2 and spin-7/2 Ising model, which was treated by Monte-Carlo simulations on a square lattice under periodic boundary conditions[8,9], investigated compensation behaviours where the global magnetization is vanished. One can compare with those behaviors tested in our model for different values of $D_A/|J|$, and $D_B/|J|$, as shown in Figs.(2,3,8(a),8(d),8(e)), respectively. It has been observed that the decrease the anisotropy of A-atoms, the decrease the transition temperature, as shown in Figs.(2,4). Whereas, a transition temperature is occurred at higher one for appropriate values of $D_A/|J| = -2.25$ and $D_B/|J| = -1.4$ (see Fig.5).

A mixed spin-3/2 and spin-7/2 Ising model [2], presented the crystal field dependence of the total magnetization M for diverse values of the temperature that M increases to its saturation value M = 1 with increasing crystal field $D/|J|$, in the presence of an external field. By contrast, it is seen that the magnetization decreases for different values of $D/|J| = -6$ as $D/|J|$ increases and it saturates to M= − 1. These results seem to be in line with ours, when the values of single-ion anisotropies for both atoms are changed, one can see Figs.(4,5). In particular, the thermal variation in the ferrimagnetically coupled system can exhibit new types of magnetization curves M, as shown in Fig.8 (a), Fig.8 (d), and Fig.8 (e), respectively. They have not been predicted in the Neel theory [15].

Such a system has not yet been done within the mean-field approximation based on the Bogoliubov inequality for the free energy. Finally, we hope that our present results may be fruitful, to support and clarify the characteristic features, in a series of molecular-based magnets $[Cr(CN)_4(\mu - CN)_2Gd(H_2O)_4 - (bpy)]_n.4nH_2O.1.5nbpy$ [2], when the experimental data of ferrimagnetic materials are analyzed.

References

1. Xu Li, Xia Long, Tian Liu, Guojun Zhu, Juexian Cao (2019) Magnetic properties and magnetic anisotropy of two-dimensional organometallic framework, Solid State Communications, 290: 22.
2. H Bouda et al (2019) Hysteresis Cycle and Magnetization Behaviors of a Mixed-Spin (7/2, 3/2) Ferrimagnetic Ising Model: Monte Carlo Investigation, J. Supercond. Magn. doi.org/10.1007/s10948-018-4981-4.
3. N De La Espriella, GM Buendía (2011) Magnetic behavior of a mixed Ising 3/2 and 5/2 spin model, J. Phys. Condens. Matter., 23: 176-003. doi:10.1088/0953-8984/23/17/176003.
4. B Deviren, M Keskin (2010) Dynamic phase transitions and compensation temperatures in a mixed spin-3/2 and spin-5/2 Ising system, J. Stat. Phys., 140: 934. doi:10.1007/s10955-010-0025-6.
5. E Albayrak (2007) The critical and compensation temperatures for the mixed spin-3/2 and spin-2 Ising model, Phys. B Condens. Matter, 391: 47-53. doi:10.1016/j.physb.2006.08.045.
6. E Albayrak (2006) Mixed spin-3/2 and spin-5/2 Ising system on the Bethe lattice, Phy. Lett. A, 353: 121.
7. OF Abubrig, D Horvath, A Bobak, M Jaščur (2001) Mean-field solution of the mixed spin-1 and 3/2 Ising system with diferent single-ion anisotropies, Physica A. 296: 437.
8. T Bahlagui, H Bouda, A El Kenz, L Bahmad, A Benyoussef (2017) Monte-Carlo simulation of compensation behavior for a mixed spin-5/2 and spin-7/2 Ising system with crystal field interaction, Super lattices and microstructures, 110: 90-97.
9. M Karimou, RA Yessoufou, GD Ngantso, F Hontinfinde, A Benyoussef (2018) Mean-Field and Monte Carlo Studies of the Magnetic Properties of a Spin-7/2 and Spin-5/2 Ising Bilayer Film, Journal of Superconductivity and Novel Magnetism, doi.org/10.1007/s10948-018-4876-4.
10. JS Da Cruz Filho, M Godoy, AS De Arruda (2013) Phase diagram of the mixed spin-2and spin-5/2 Ising system with two different single-ion anisotropies, Physica A 392: 62-47.
11. JS Da Cruz Filho, TM Tunes, M Godoy, AS De Arruda (2016) Effects of two different random single-ion anisotropies on the critical properties of a *mixed spin-2* and *spin-5/2* Ising system, Physical A, 450: 180.
12. A Dakhama, N Benayad (2000) On the existence of compensation temperature in 2d mixed-spin Ising ferrimagnets: an exactly solvable model, J. Magn. Magn. Mater., 213: 117.

13. B Deviren, M Keskin, O Canko (2009) Magnetic properties of an anti-ferromagnetic and ferrimagnetic mixed spin-1/2 and spin-5/2 Ising model in the longitudinal magnetic field within the effective-field approximation, Phys. A: Stat. Mech. Its Appl., 388: 1835-1848. doi:https://doi.org/10.1016/j.physa.2009.01.032.

14. N De La Espriella, CA Mercado, JC Madera (2016) Spin compensation temperatures in the Monte Carlo study of a *mixed spin-2 and spin-5/2* Ising ferrimagnetic system, Magn. Magn. Mater., 401: 22.

15. L Néel (1948) Magnetic properties of ferrites: ferrimagnetism and anti-ferromagnetism, Ann. Phys., 3: 137.

16. T Kaneyoshi, M Jascur (1993) Magnetic properties of a ferromagnetic or ferrimagnetic bilayer system, Physical a 195: 474.

