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RESEARCH ARTICLE

Magnetic and thermodynamic properties of a mixed spin-1and spin-7/2 Blume-Capel Ising ferrimagnetic system

Hadey K. Mohamad
Dept. of Physics, College of Science, Al-Muthanna University, Samawa, Iraq.

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***Corresponding Author**

Hadey K. Mohamad

Abstract

The magnetic properties of a mixed-spin Blume-Capel Ising ferrimagnetic system are investigated. It has been studied the effect of the crystal field and longitudinal magnetic field on the magnetic properties and thermodynamic quantities of the system, respectively. So, it has been calculated Gibbs free energy of the mixed spin ferrimagnetic model such that the total magnetizations and compensation points have been examined by minimizing the free energy based on the Bogoliubov inequality. A mixed spin-1 and spin-7/2 ferrimagnet with different single-ion anisotropies, i.e., crystal fields on a square lattice, is investigated. It has been used a mean field method and found that the crystal-field interaction plays an important role in the existence and induction of compensation points. Some outstanding behaviors in the temperature dependences of total magnetizations in the presence of longitudinal fields have been shown as well.

Introduction

Magnetic solids have numerous and important technological applications: they find wide use in information storage devices, microwave communications systems, electric power transformers and dynamos, and high-fidelity speakers[1,2]. By far the largest application of magnetic materials is in information storage media, and the annual sales of computer diskettes, compact disks, optical disks, recording tape, and related items exceed those of the celebrated semiconductor industry[3,4]. In response to the increasing demands being placed on the performance of magnetic solids, over the last decade or so there has been a surge of interest in molecule-based magnets[5-8]. In recent years, most research attention has been directed to the mixed spin system having spin-1 and spin-S(S>1) with a crystal field interaction. So, some researchers have worked on mixed-spin Blume-Capel Ising systems where both constituents have spin values larger than 1/2. It has been investigated by a variety of techniques such as exact, mean-field approximation, and effective field theory[9-17]. The aim of this paper is to study the effects of anisotropies, i.e., crystal fields , longitudinal ones on the transition temperatures, and magnetization curves, respectively, in the molecular-based magnetic systems of the first-neighbor interaction for a mixed spin-1 and spin-7/2 Ising model on square lattice. This study is done by the use of mean-field approximation based on the Bogoliubov inequality for Gibbs free energy. The present work may study the spin compensation temperature of the system can be obtained by requiring the total magnetization as being equal to zero for various values of crystal fields; though the reduced magnetization of the sublattices forming the system are not equal to zero[13-18]. In this correspondence we are concerned to study the phase diagrams(magnetization and compensation points), and examine the thermodynamic quantities of the mixed spin ferrimagnetic Blume-Capel Ising system with various values of the crystal fields.

2. Theoretical framework:

The model which is considered, consists of two-dimensional sublattices $\sigma_i^{\,A}$ and $S_j^{\,B}$. The sites of $\sigma_i^{\,A}$ are occupied by A-atoms with the fixed spin σ_i. The sites of $S_j^{\,B}$ occupied by B-atoms with the spin S_j. The system is described by the following Hamiltonian :

$$H = -\sum_{i,j} J_{ij}\sigma_i^A s_j^B - D_A\sum_i(\sigma_i^A)^2 - D_B\sum_j(s_j^B)^2 - h\sum_{i,j}(\sigma_i^A + S_j^B) \qquad (1)$$

where $\sigma_i^{\,A} = 0,\pm1$, $S_j^{\,B} = \pm1/2,\pm3/2,\pm5/2,\pm7/2$ and $J_{ij} < 0$. D_A, D_B are the anisotropies, i.e., crystal fields acting on the spin-1 and spin-7/2 respectively. J_{ij} is the exchange interaction between spins at sites i and j .

The approximated free energy of the system considered is obtained from a variational method based on Bogoliubov inequality[13,19], that

$$F(H) \le F(H_O) + \langle H - H_O \rangle \qquad (2)$$

$F(H)$ is the free energy of Hamiltonian , $F(H_O)$ is the free energy of a trial Hamiltonian, that :

$$F(H) = -\beta^{-1}\ln Z \; ; F(H_o) = \beta^{-1}\ln Z_o \qquad (3)$$

Z stands for the partition function of the system which is defined as

$$Z = \sum_{i,j} e^{-\beta H} \qquad (4)$$

Thus, the free energy per spin, has the form:

$$f = -\frac{1}{2\beta}\{\ln[1+2e^{\beta D_A}\cosh(\beta\lambda_A + H^o)] + \ln[2e^{49/4\beta D_B}\cosh(\frac{7}{2}\beta\lambda_B + H^o)$$
$$+2e^{25/4\beta D_B}\cosh(\frac{5}{2}\beta\lambda_B + H^o) + 2e^{9/4\beta D_B}\cosh(\frac{3}{2}\beta\lambda_B + H^o) + 2e^{1/4\beta D_B}\cosh(\frac{1}{2}\beta\lambda_B + H^o)]\}$$
$$+1/2(-zJm_Am_B + \lambda_A m_A + \lambda_B m_B)$$
(5)

where $\beta = \frac{1}{K_B T}$, $H^o = \beta h$, and z(z=4) its nearest-neighbor coordination number of a square lattice.

Minimizing this expression with respect to λ_A and λ_B gives self-consistent expressions for the mean-field as follows:

$$\lambda_A = zJm_B \quad , \lambda_B = zJm_A \quad , \qquad (6)$$

with,

$$m_A \equiv \left\langle \sigma_i^A \right\rangle_o = \frac{2\sinh a}{2\cosh a + e^{-\beta D_A}} \; , \qquad (7)$$

$$m_B \equiv \left\langle S_j^B \right\rangle_o = \frac{1}{2}\frac{7\sinh(\frac{7}{2}b)+5e^{-6\beta D_B}\sinh(\frac{5}{2}b)+3e^{-10\beta D_B}\sinh(\frac{3}{2}b)+e^{-12\beta D_B}\sinh(\frac{1}{2}b)}{\cosh(\frac{7}{2}b)+e^{-6\beta D_B}\cosh(\frac{5}{2}b)+e^{-10\beta D_B}\cosh(\frac{3}{2}b)+e^{-12\beta D_B}\cosh(\frac{1}{2}b)}$$

(8)

where

$a = \beta zJm_B + \mathrm{H}; b = \beta zJm_A + \mathrm{H}$.

It is worth to note that the ferrimagnetic case shows the signs of sublattice magnetizations are different, and there may be a compensation point, at which the total magnetization per site equals to zero, that:

$$M = \frac{1}{2}(m_A + m_B) \quad ; (m_A = -m_B \neq 0) \tag{9}$$

3. Results and discussions :

First, we have investigated the phase diagrams of the system which can be determined from the sublattice magnetizations of a mixed spin-1 and spin-7/2 Blume-Capel Ising model(Eqs.(4),(5),(6)). At zero temperature, one can find eight phases with different values of { m_A, m_B, Q_A, Q_B }, namely, the ordered ferrimagnetic phases

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

and there are disordered phases

$$D_1 = (0,\frac{7}{2}), or(0,-\frac{7}{2}), D_1(0,\frac{5}{2}), or(0,-\frac{5}{2}), D_3(0,\frac{3}{2}), or(0,-\frac{3}{2}), D_4(0,\frac{1}{2}), or(0,-\frac{1}{2}) ,$$

where the parameters Q_A and Q_B are defined by

$$Q_A = \left\langle (\sigma_i^A)^2 \right\rangle, \qquad Q_B = \left\langle (S_j^B)^2 \right\rangle \tag{10}$$

let us consider the case when $-1.999 \leq D_B/|J| \leq -1.95$. Fig.(1) stands for the low-temperature dependences of magnetization for the mixed-spin Blume-Capel Ising Ferrimagnet on a square lattice(z=4), with a fixed value of $D_A/|J| = -2.0$. One can observe characteristic behaviours of compensation transitions at different values of $D_B/|J|$.

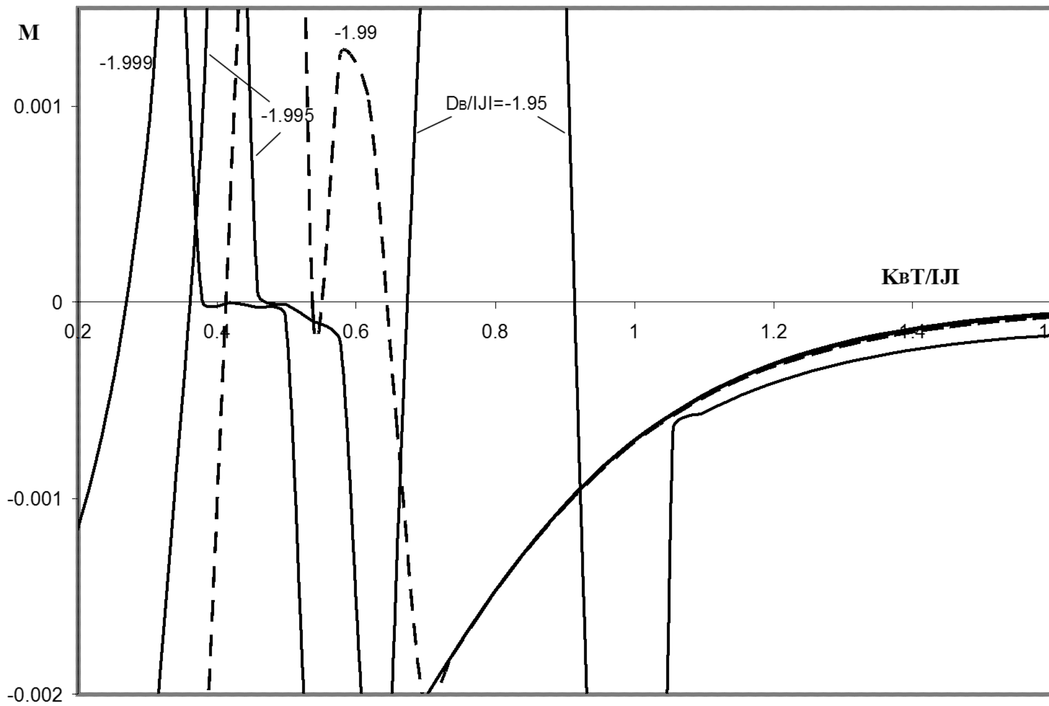


Fig.1. Thermal variations of the total magnetization M for the mixed spin Blume-Capel Ising ferrimagnet with the coordination number z=4,when the value of $D_B/|J|$ is changed , for fixed $D_A/|J| = -2.0$, $h/|J| = 0.0$.

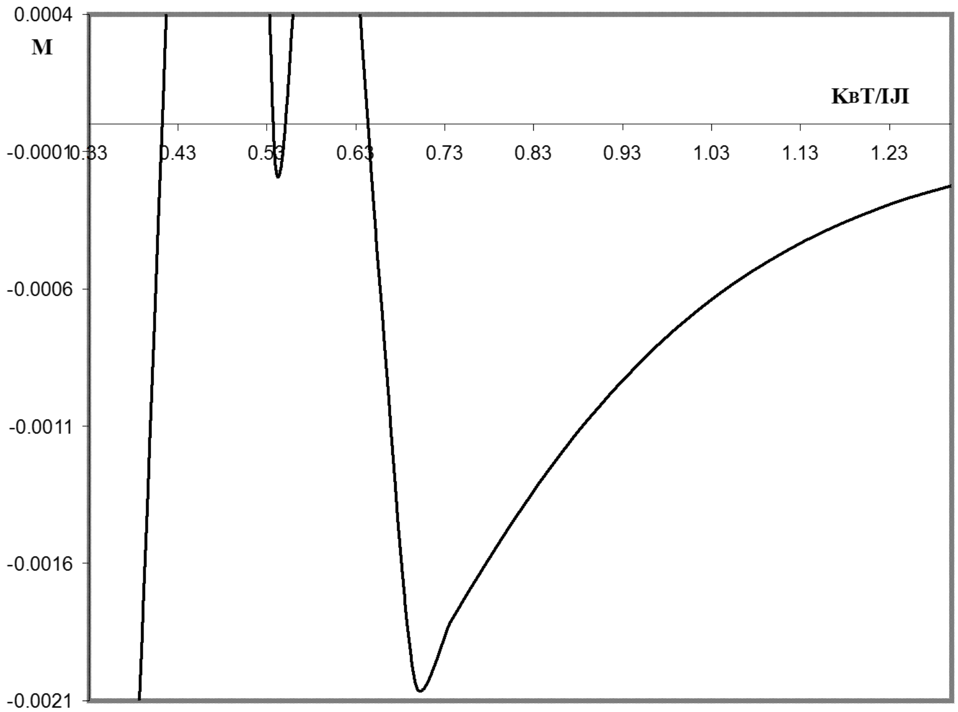


Fig.2. A close view the temperature dependences of the magnetization for the mixed-spin Blume-Capel Ising ferrimagnet with the coordination number z=4, when $D_B/|J| = -1.99$ and $D_A/|J| = -2.0$.

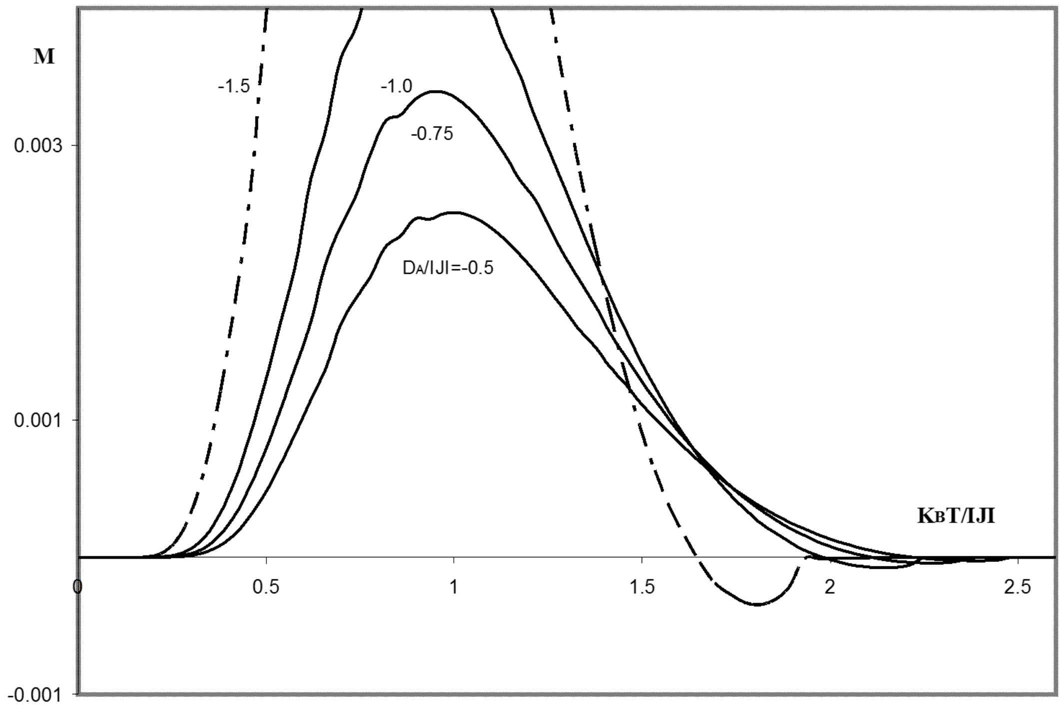


Fig.3. Thermal variations of the total magnetization M for the mixed spin Blume-Capel Ising ferrimagnet with the coordination number z=4,when the value of $D_A/|J|$ is changed , for fixed $D_B/|J| = -2.0$, $h/|J| = 0.0$.

Fig.(2) expresses a close view low-temperature phase diagram for the mixed spin ferrimagnet with the coordination number z=4, at $D_A/|J| = -2.0$, $D_B/|J| = -1.99$, in the absence of magnetic field, indicating a possibility of many compensation temperatures. Thus, the system considered may exhibit an interesting thermal variation behaviour(w-type)[20].

On the other hand, one can observe characteristic features of compensation transitions at different values of $D_A/|J|$, for a fixed value of $D_B/|J| = -2.0$, as in Fig.3, where the system may show two compensation temperatures at $T = 0K^o$, and at $T \neq 0K^o$, respectively.

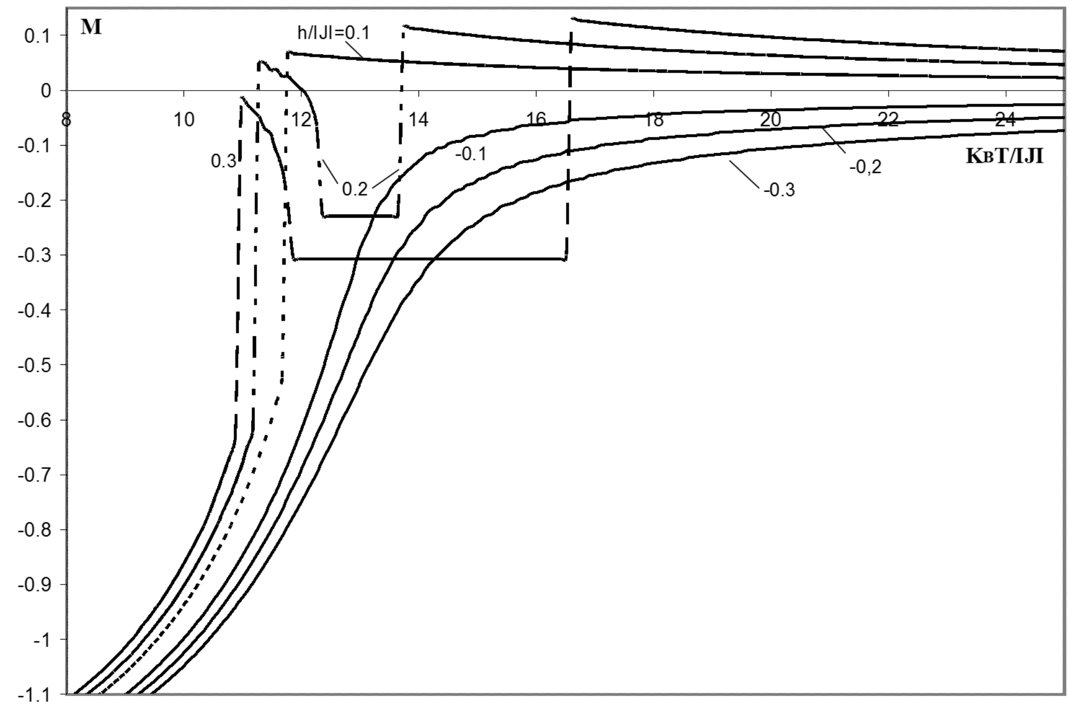


Fig.4. The temperature dependences of the total magnetizations M for the mixed–spin Blume-Capel Ising ferrimagnet with the coordination number z=4.0 ,when $D_A/|J| = D_B/|J| = 10$, with various values of $h/|J|$.

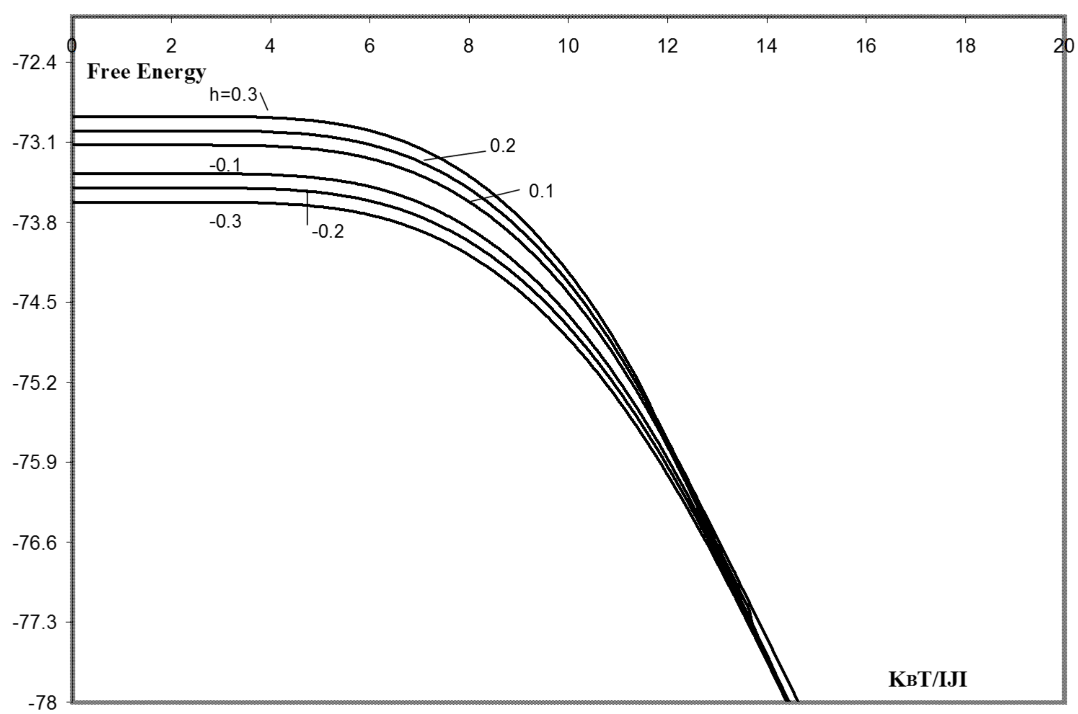


Fig.5. The temperature dependencies of free energy G for the mixed spin Blume-Capel Ising ferrimagnet with the coordination number z=4,when the value of $h/|J|$ is changed , for fixed $D_A/|J| = D_B/|J| = 10.0$.

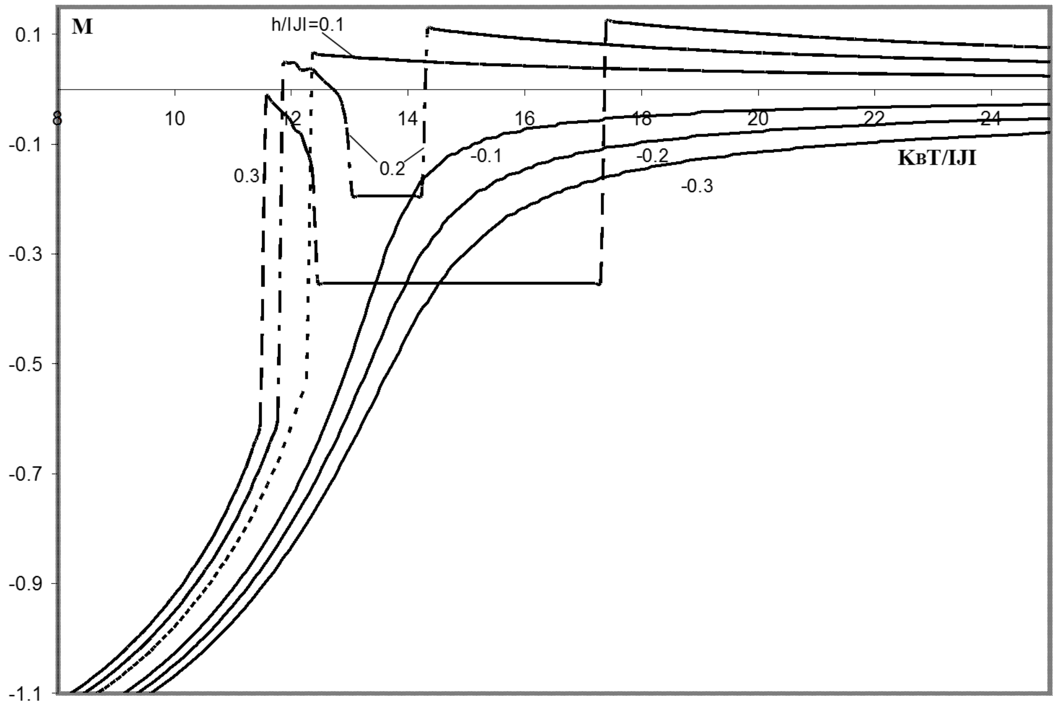


Fig.6. The temperature dependences of the total magnetizations M for the mixed–spin Blume-Capel Ising ferrimagnet with the coordination number z=4.0 ,when $D_A/|J| = D_B/|J| = 20$, with various values of $h/|J|$.

In the presence of an external magnetic field, the system, as shown from Figs.((4),(6)) may exhibit three compensation point in the thermal variation of the system magnetization, which can be obtained by solving the coupled equations for m_A and m_B numerically[13,19], depending on the values of the external magnetic fields in the range of values of interest for longitudinal fields, when $-0.3 \le h/|J| \le 0.3$, with two different values of crystal fields $D_A/|J| = D_B/|J| = 10.0, 20.0$, acting on the A atoms and B atoms, respectively. In the region where the mixed-spin system may show a compensation point, the sublattice magnetization m_B is more ordered than the sublattice magnetization m_A below compensation temperature T_K, that is, $|m_B| > |m_A|$ (see Figs.(1),(2),(3),(4),(6)). These sublattice magnetizations is still incomplete($m_A \ne -m_B$), so there is a residual magnetization in the system($M \ne 0$).This is due to the antiferromagnetic nearest-neighbor interaction which tends to align neighboring spins in opposite directions. As the temperature is increased, at certain values of crystal fields D_A, D_B acting on the A-atoms and B-atoms, respectively, the direction of this residual magnetization may switch[17,18]. Now, let us examine the contribution of free energy to the thermodynamic phase stability of the mixed spin ferrimagnet which is considered. Gibbs free energy as a function of temperature has been calculated according to Eq.(5), is shown in Figs.((5),(7)). For description of the free energy of the ferrimagnet(at compensation point) and paramagnet(at transition temperature), one can observe the free energy curves have an inflexion that it corresponds a discontinuous behaviour, and at critical temperature the free energy of the system is continuous, respectively. The results shown in Figs.((5),(7)) are consistent with those derived from Figs.((4),(6)).

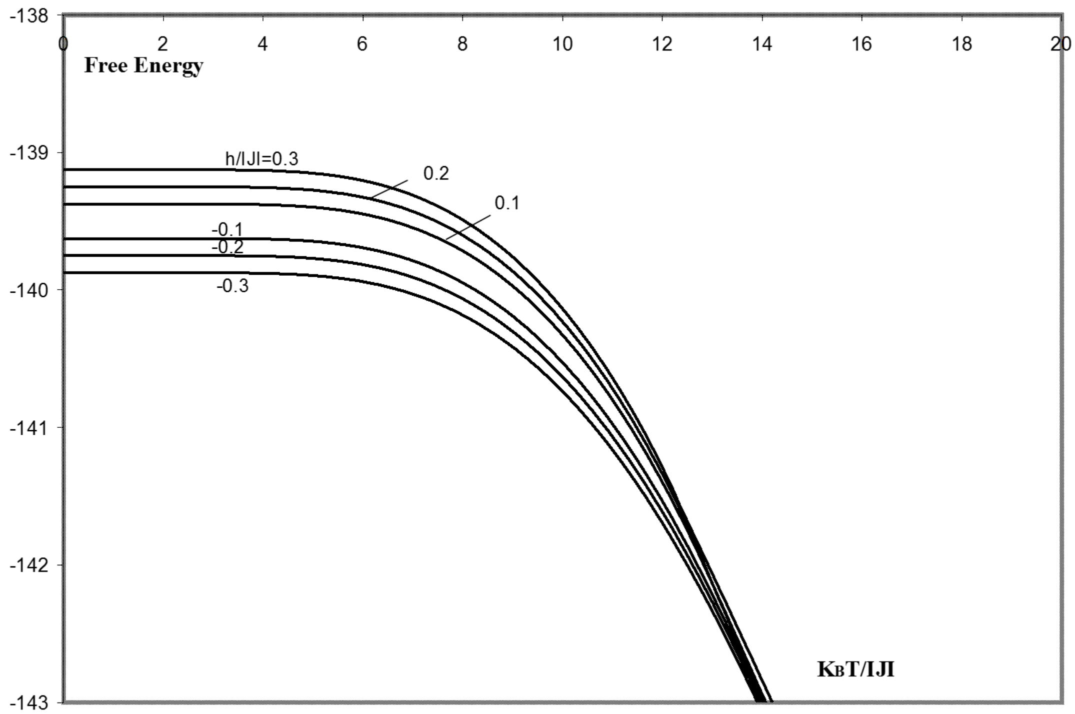


Fig.7. The temperature dependencies of free energy G for the mixed spin Blume-Capel Ising ferrimagnet with the coordination number z=4,when the value of $h/|J|$ is changed , for fixed $D_A/|J| = D_B/|J| = 20.0$.

It is interesting to examine the characteristic properties of the system. We find the compensation temperature (T_k) depends strongly on the values of longitudinal magnetic fields and crystal fields D_A, D_B acting on the $A-$ atoms and $B-$ ones, respectively. From Fig.(8), the computed partition function of the system considered $\ln Z$ (Eq.(4)), for $h/|J| = 0$, is shown for various crystal fields $D_B/|J| = -1.95, -1.99, -1.995, -1.999$. In this case only the finite curves connected with the spin compensation temperature are seen. For $h/|J| > 0$ the partition function diverges at $T = 0K^o$, which is connected with the rapid rearrangement of the ground state from $m_A = 1$, $m_B = -7/2$ configuration to the configuration characterized by $m_A = -m_B \le 0.5$, which occurs for $0.1 \le h/|J| \le 0.3$, at $T > 0K^o$ (see Figs.((9),(10)).

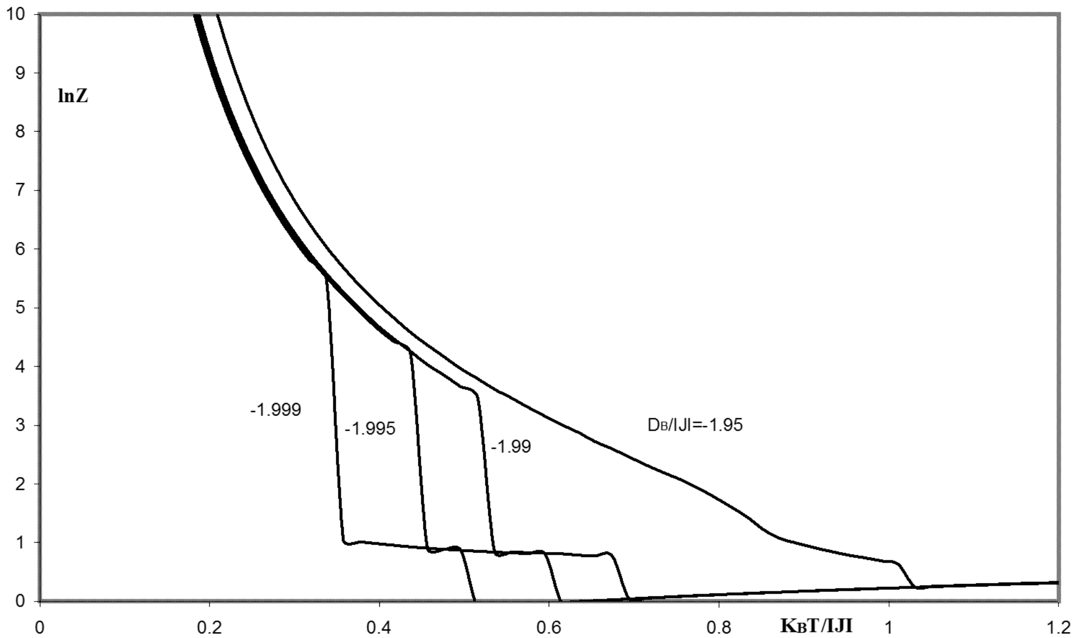
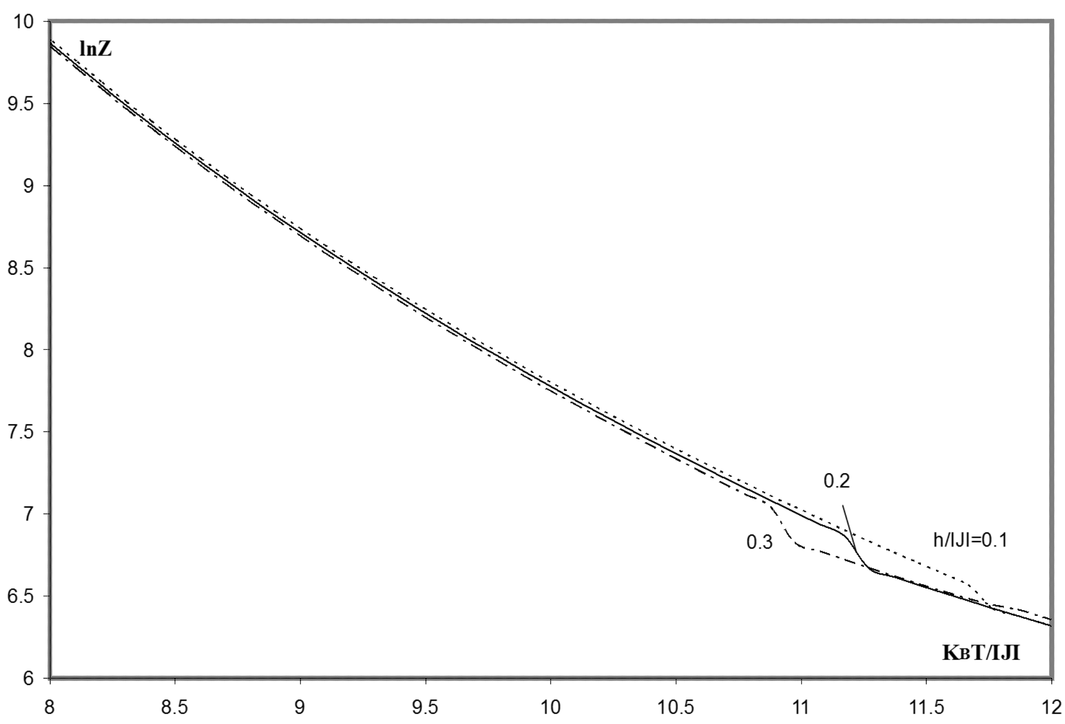


Fig.8. The temperature dependences of partition function lnZ for the mixed spin Blume-Capel Ising ferrimagnet with the coordination number z=4,when the value of $D_B/|J|$ is changed , for fixed $D_A/|J| = -2.0$, $h/|J| = 0.0$.



. Fig.9. The temperature dependences of partition function lnZ for the mixed spin Blume-Capel Ising ferrimagnet with the coordination number z=4,when the value of $h/\left|J\right|$ is changed , for fixed $D_A/\left|J\right| = D_B/\left|J\right| = 10.0$.

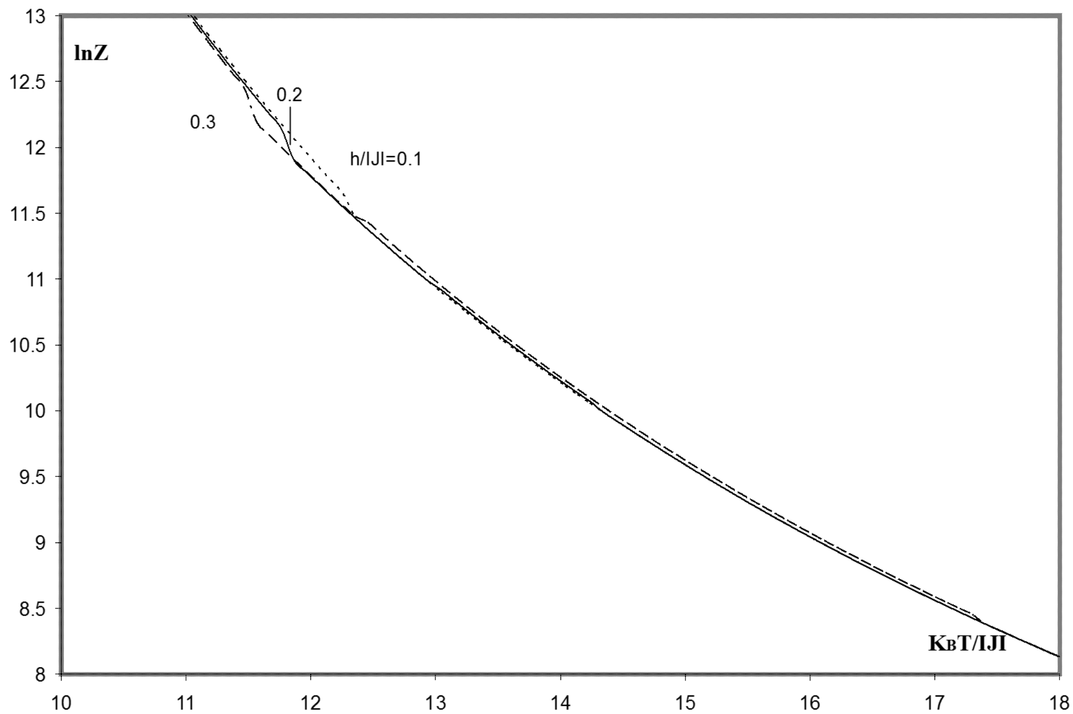


Fig.10. The temperature dependences of partition function lnZ for the mixed spin Blume-Capel Ising ferrimagnet with the coordination number z=4,when the value of $h/\left|J\right|$ is changed , for fixed $D_A/\left|J\right| = D_B/\left|J\right| = 20.0$.

4.Conclusions :

The mean-field approximation has been used in this treatment . The phase diagram of the mixed spin-1 and spin-7/2 Blume-Capel Ising Ferrimagnetic system with different single-ion anisotropies, i.e., crystal fields, has been investigated. The magnetic and thermodynamic properties of the system with different crystal fields and longitudinal ones have been found by solving the general expressions numerically. So, the magnetization curves have exhibited some characteristics, that it has been shown the mixed-spin ferrimagnetic system which is considered may exhibit an outstanding feature(many compensation points). One can compare our results with those of a mixed spin-1 and spin-3/2 system[21], and mixed spin-1/2 and spin-5/2 within the effective field approximation[16], in which the mixed-spin model shows two or three compensation temperatures depending on the values of the crystal fields, respectively. It is worth to note that our model may exhibit four compensation points. One should notice that a new behaviour not predicted in the Ne'el theory of ferrimagnetism[11]. A theoretical study dealing with the mixed spin-2 and spin-5/2 Ising model, using MFA[13], indicated that the possibility of many compensation points is found when the crystal fields acting on both atoms increase. These results seem to be in line with ours, when the value of D_B is changed, for a fixed value of D_A, as shown in Figs.((1),(2)). In addition to this, the mixed-spin Blume-Capel Ising system considered may exhibit interesting behaviours in which case a transition temperature is examined. So, we have observed that the decrease the crystal field of B-atoms the decrease the transition temperature, as shown in Fig.(3). Whereas, under the influence of the external magnetic fields, a transition temperature is occurred at higher one for appropriate values of $D_A/|J| = D_B/|J| = 10.0, 20.0$, respectively(see Figs.4,6). It remains to mention that the partition functions for two dimensional nearest neighbour Blume-Capel Ising models have been computed for square lattice(z=4), in the absence and presence of a magnetic field. So, the thermodynamic quantities of the mixed spin ferrimagnetic Blume-Capel Ising system with various values of the crystal fields and longitudinal ones have been examined(see Figs.(8),(9),(10)). Finally, we hope that our present results may be helpful to support and clarify the characteristic features, for a square lattice, in a series of molecular-based magnets, when the experimental data of ferrimagnetic materials are analyzed .

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