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Oguchi Approximation of a mixed spin-2 and spin-5/2 Blume-Capel Ising ferrimagnetic system

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Abstract- By using the Oguchi approximation(OA), we study a mixed spin-2 and spin-5/2 Blume-Capel Ising ferrimagnet with different single-ion anisotropies on a simple cubic lattice. It has been carried out Oguchi method and calculated the free energy of a mixed spin ferrimagnetic model from the partition function. By minimizing the free energy, it has been obtained the equilibrium magnetizations and the compensation temperatures. The existence and dependence of a compensation temperature on the crystal field is mainly investigated.

Index Terms- Mixed-spin Blume-Capel Ising model; Oguchi approximation; Ferrimagnet; Crystal field; Compensation points.

I. INTRODUCTION

Recently, a lot of efforts has been directed to the ferrimagnetic materials, specially due to their great potential for technological applications [1,2]. In a ferrimagnetic material two inequivalent moments, interacting antiferromagnetically, can give rise to a zero spontaneous magnetization below its critical temperature[3]. Then, a special point which is called spin compensation temperature can appear at a temperature below the critical one (T_c), where the sublattice magnetizations cancel exactly each other[4-8]. T. Kaneyoshi et al have proposed that a diluted mixed spin-2 and spin-5/2 ferrimagnetic Ising system on honeycomb lattice can explain the characteristic temperature dependence of magnetization observed at low temperatures in the molecular-based magnetic material, $AFe^{II}Fe^{III}(C_2O_4)_3[A = N(n-C_nH_{2n+1})_4, n = 3-5]$[9]. Y. Nakamura et al observed that the effect of external magnetic fields on the lattice possibly leads to a compensation transition[10]. The authors of [11], in this respect, investigated the magnetic properties of a mixed spin-2 and spin-5/2 Ising ferrimagnetic system in the phase diagram and in the compensation temperature. It is worth to note that a mixed-spin Ising ferrimagnetic system on a simple cubic lattice in which the two mixing sublattices have spins two ($0,\pm1,\pm2$) and spins five-half($\pm1/2,\pm3/2,\pm5/2$), has not been examined within Oguchi approximation(OA). So, instead of using the decoupling approximation, we have introduced the concept of a correlation behaviour to understand the corporative effects exhibited by such systems. We found that the system considered exhibits the compensation phenomenon at low temperatures. Our results show the possibility of many compensation points at low temperatures depending on certain values of anisotropies near by the boundaries of order-phase transitions in the ground-state structure of the system.

II. THEORY

The mixed-spin ferrimagnetic Ising model, which is considered, consists of three-dimensional sublattices S_i and S_j with spins $S_i^A = 0,\pm1,\pm2$ and $S_j^B = \pm1/2,\pm3/2,\pm5/2$ respectively. In this research, the system is described by the Oguchi approximation[12], that:

$$H = -JS_i^A S_j^B - D_A\sum_i (S_i^A)^2 - D_B\sum_j (s_j^B)^2 - (h_i S_i^A + h_j S_j^B) \quad (1)$$

with,

$$h_i = J(z-1)m_B \;, \quad h_j = J(z-1)m_A$$

where , and $J<0$. J is the exchange interaction between spins at sites i and j. z is the number of nearest neighbouring spins and the sublattice magnetizations m_A and m_B are the thermal averages of S_i^A and S_j^B, respectively, i.e., $m_A = <S_i^A>$, and $m_B = <S_j^B>$. Taking the eigenvalues of the Hamiltonian(1), one can obtain the sublattice magnetizations per site (Appendix I). D_A, D_B are the anisotropies, i.e., the crystal fields, acting on the spin-2 and spin-5/2 respectively.

The knowledge of the partition function(Z) allows to express the relations for thermodynamic quantities. Then, the free energy of the model is defined as[13],

$$F \equiv -k_B T \ln Z \;; \quad Z = \sum_{i,j} e^{-\beta H} \quad (2)$$

where F is the free energy of H given by relation (1), $\beta = \frac{1}{K_B T}$. The sublattice magnetization per site is obtained by minimizing the free energy (Eq.2) which is given by Appendix 1. It is worth noting that the ferrimagnetic case shows that the signs of sublattice magnetizations are different, and there may be a compensation point at which the total longitudinal magnetization per site[11,14], that

$$M = \frac{1}{2}(m_A + m_B)$$

is equal to zero.

III. Results and Discussions

In this work, we examine the magnetic properties concerning spin compensation temperatures of the three-dimensional mixed spin-2 and spin-5/2 ferrimagnetic Blume-Capel Ising model. First, let us study the phase diagram of the mixed-spin ferrimagnetic system with different crystal fields through which, we interest to consider the characteristic magnetic properties of the system.

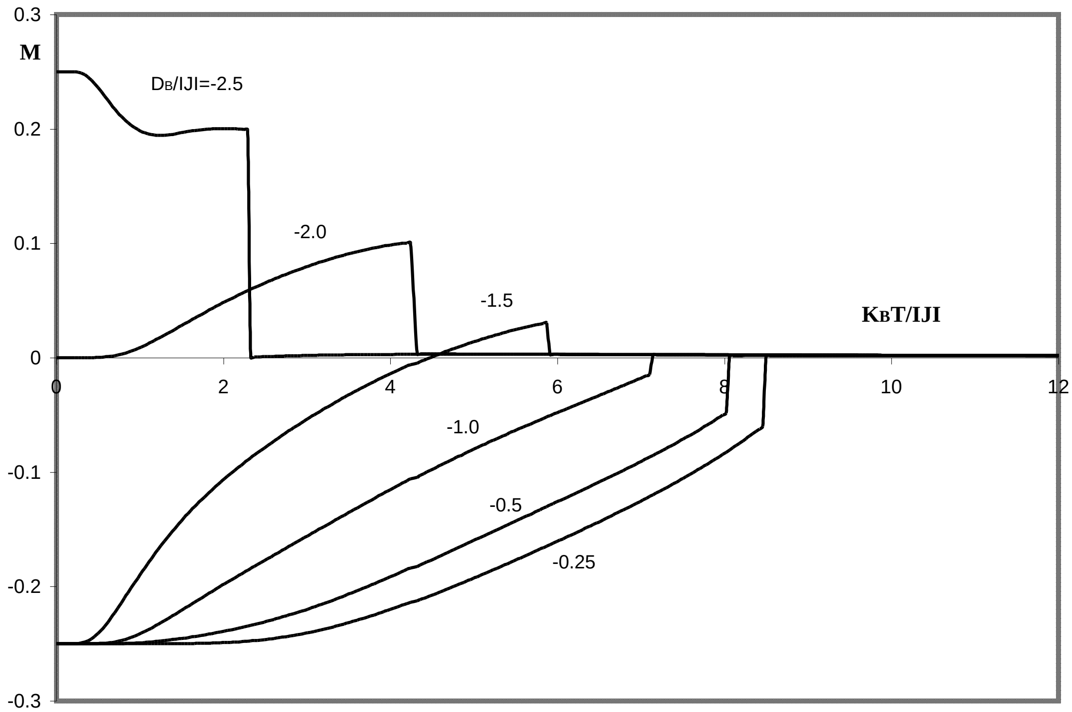

Fig.1. Thermal variations of the total magnetizations M for the mixed–spin Blume-Capel Ising ferrimagnet with the coordination number z=6.0 ,when $D_A/|J| = -1.0$, with various values of $D_B/|J|$.

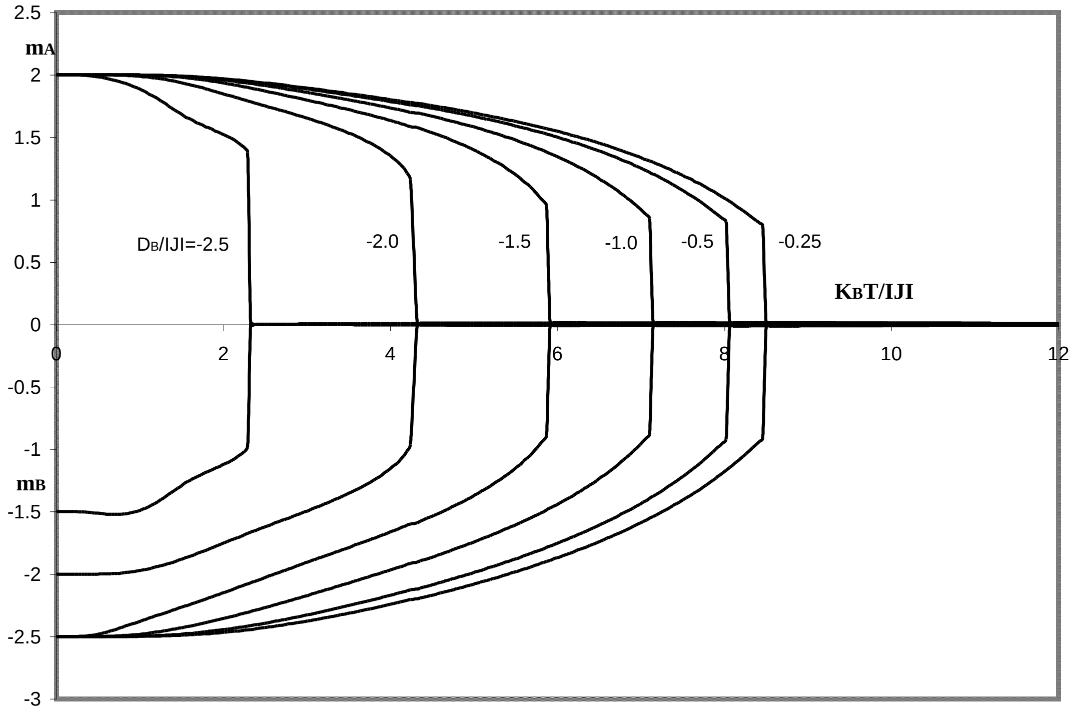

Fig.2. Thermal variations of the sublattice magnetizations for the mixed–spin Blume-Capel Ising ferrimagnet with the coordination number z=6.0 ,when $D_A/|J| = -1.0$, with various values of $D_B/|J|$.

Fig.(1), and Fig.(2) stand for the total magnetization and sublattice magnetizations versus the absolute temperature for the values of $D_A/|J| = -1.0$, respectively. As shown in the figures, the system may exhibit one compensation point in the phase diagrams depending on the values of crystal fields($D_B|J|$), in the range $-2.5 \leq D_B|J| \leq -0.25$. We report an interesting feature of compensation temperatures for $D_A/|J| = -1.0$, and for the value $D_B/|J| = -1.5$. The result shown in the Fig.(3) is consistent with that derived from Fig.(2). As is seen from the figure, in the region where the system may show a compensation point, the spin-2 sublattice magnetization is more ordered than the spin-5/2 sublattice magnetization below the compensation temperature. As the system is heated up, the direction of residual magnetization may switch. That is to say, due to entropy some spins can flip their directions[2]. Thus, the spin-5/2 sublattice magnetization becomes more ordered than the spin-2 sublattice magnetization for temperatures above the compensation temperature. So there is an intermediate temperature such that the cancellation is complete($M = 0$)[11,14].

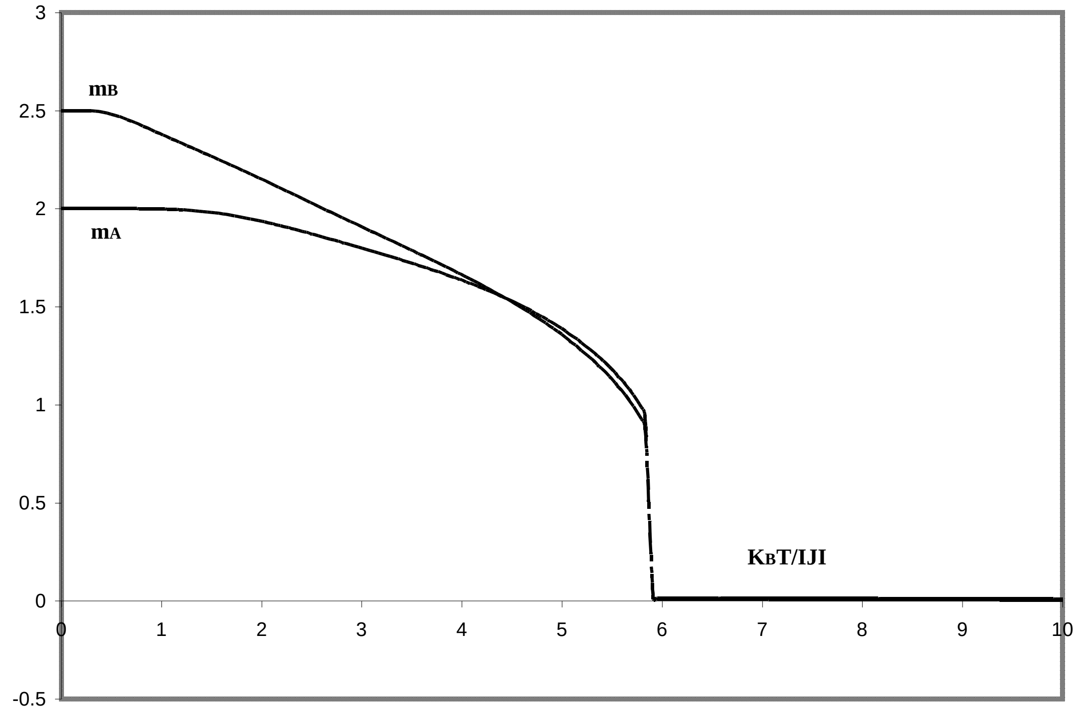

Fig.3. Thermal variations of the sublattice magnetizations for the mixed–spin Blume-Capel Ising ferrimagnet with the coordination number z=6.0 ,when $D_A/|J| = -1.0$ **, and** $D_B/|J| = -1.5$ **.**

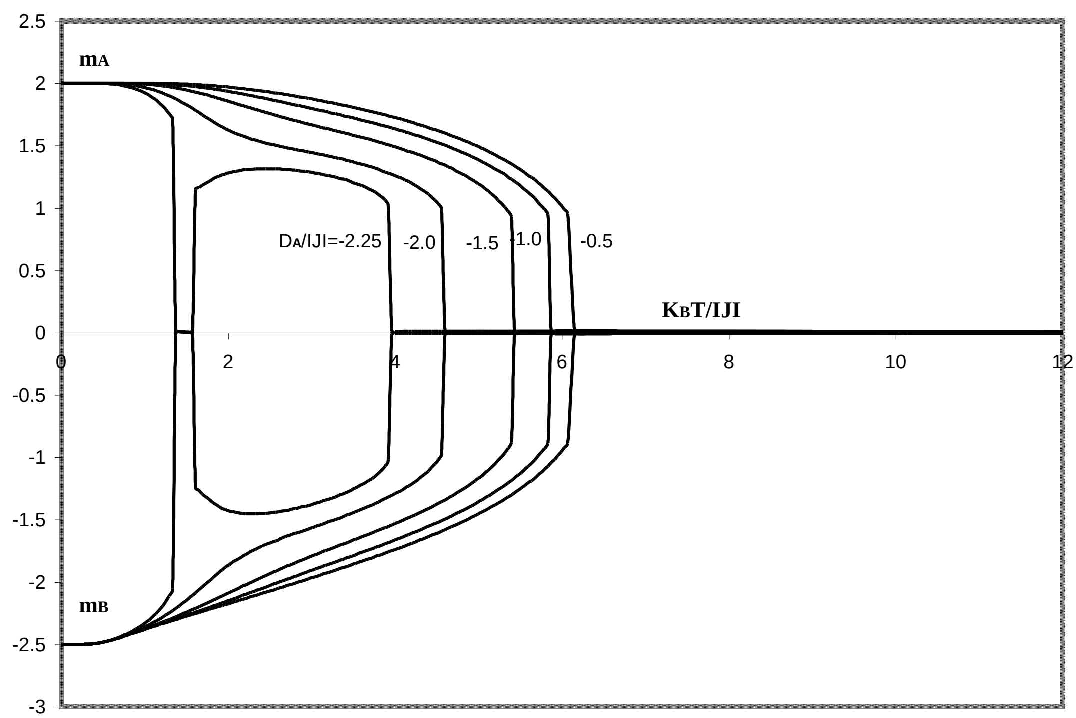

Fig.4. Thermal variations of the sublattice magnetizations for the mixed–spin Blume-Capel Ising ferrimagnet with the coordination number z=6.0 ,when $D_B/|J| = -1.5$, with various values of $D_A/|J|$.

Fig(4) expresses the characteristic behaviours of m_A, m_B as a function of $k_B T$ for different values of $D_A/|J| = -2.25, -2.0, -1.5, -1.0, -0.5$, where the system may exhibit three or many compensation temperatures, when $D_A/|J| = -2.25$, and $D_B/|J| = -1.5$. Our results are obtained in a microscopic model describing the magnetic behaviors of this mixed-spin system that shows remarkable insight compared to[9,10]. It is worth noting that we have introduced the concept of a correlation behaviour. As is seen in Figs.((4),(5)), when the value of the negative crystal field on A-atoms is relatively large, a compensation point may be existed. So, the possibility of many compensation points is found when the negative crystal fields acting on A-atoms increase. The author of [9] investigated the mixed spin-5/2 and spin-2 Ising model on a honeycomb lattice, which may exhibit a compensation point when the value of the positive single-ion anisotropy, i.e., the crystal field on B-atoms(spin-2) is relatively large in the layered system on the basis of MC simulation. Whereas, the effective-field approximation predicts the existence of a compensation temperature, but only for relatively small transverse fields, in the absence of crystal field[10]. One can compare our results with that ones published in refs.[9,10].

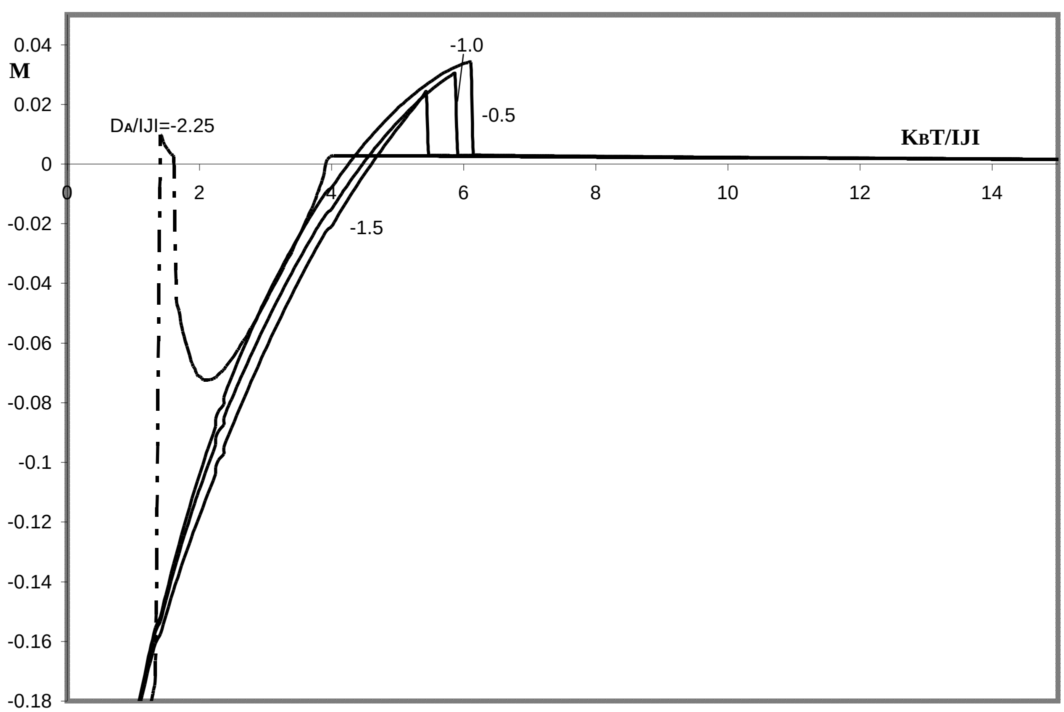

Fig.5.The temperature dependences of the total magnetization M for the mixed –spin Blume-Capel Ising ferrimagnet with the coordination number z=6.0, when $D_B/|J| = -1.5$, with various values of $D_A/|J|$.

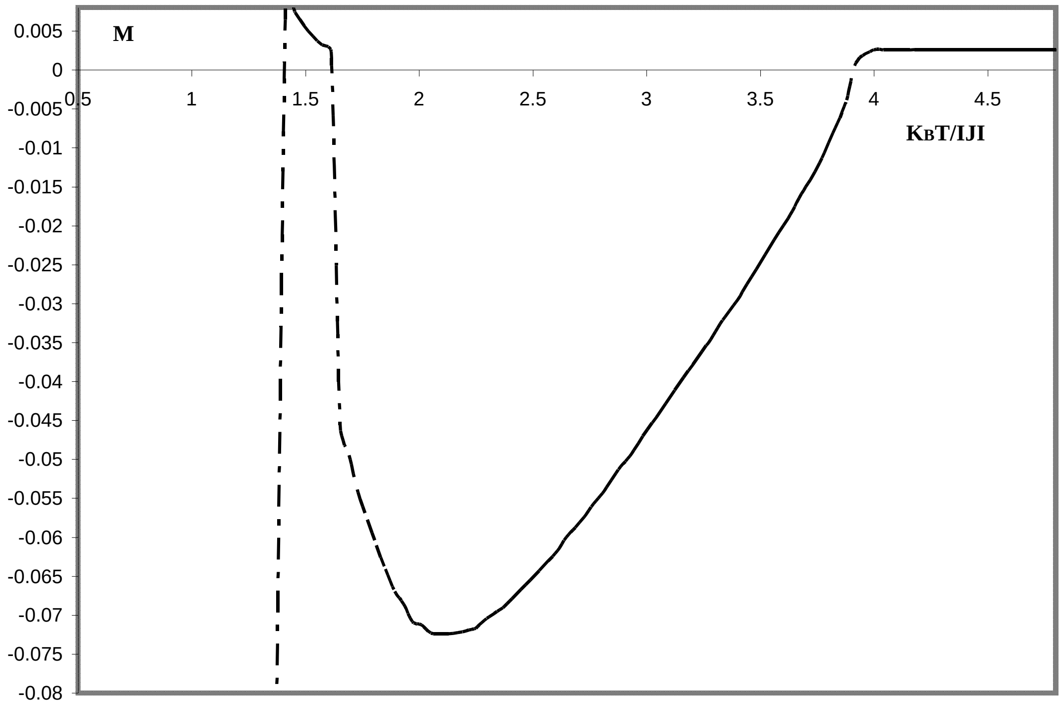

Fig.6. A close view of the temperature dependence of the total magnetization M for the mixed–spin Blume-Capel Ising ferrimagnet with the coordination number z=6.0, when $D_B/|J| = -1.5$, and $D_A/|J| = -2.25$

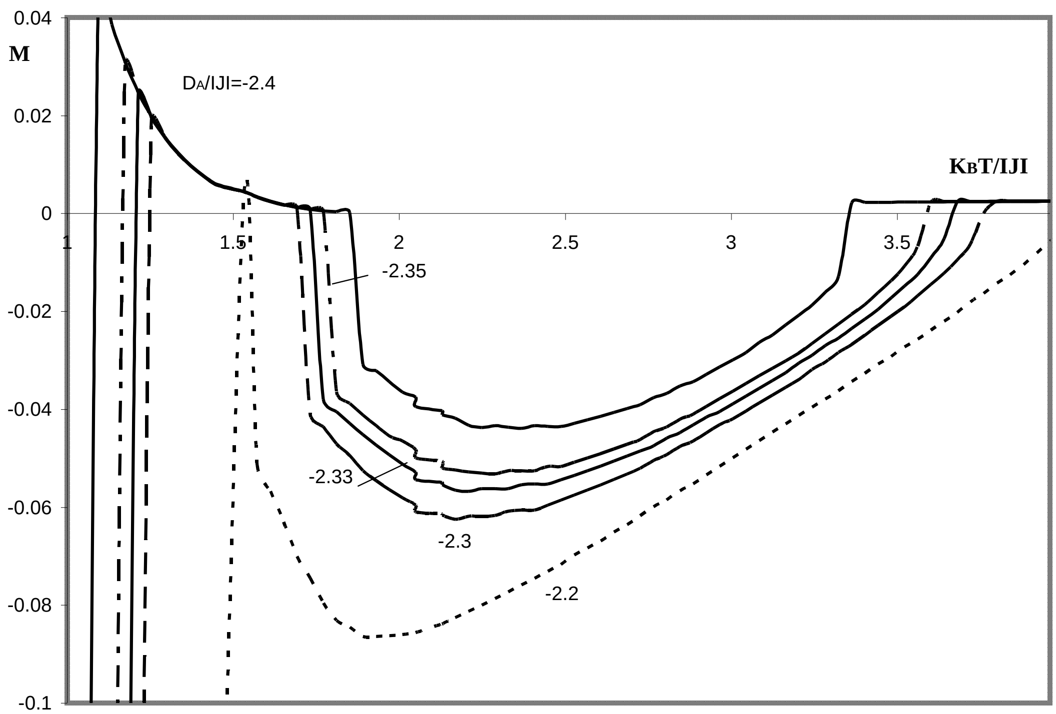

Fig.7. The temperature dependences of the total magnetizations M for the mixed–spin Blume-Capel Ising ferrimagnet with the coordination number z=6.0 ,when $D_B/|J| = -1.5$, with various values of $D_A/|J|$.

Fig.(5) may show a characteristic feature for the temperature dependencies of M in the system for different values of crystal fields acting on A-atoms, with a fixed one of $D_B/|J| = -1.5$. Fig.(6) expresses a close view of the compensation behaviour derived from Fig.(5), for the mixed–spin Blume-Capel Ising ferrimagnet with the coordination number z=6.0, when $D_B/|J| = -1.5$, and $D_A/|J| = -2.25$.

Now, let us examine the system in the range $-2.4 \le D_A|J| \le -2.2$. As is seen from the Fig.(7), the present system may clearly exhibit many compensation points for the M curves labeled $D_B/|J| = -1.5$, with different values of D_A, at $T \neq 0$, which is classified after Neel as the W-type[1]. One can compare our results with those obtained in the mixed spin-2 and spin-5/2 systems[9,15], in which the models show one compensation temperature, respectively. Also, we find that the transition (or critical) temperature depends strongly on the values of anisotropies D_A, D_B acting on the A-atoms and B-atoms, respectively, where the transition temperature can be determined by requiring that the sublattice magnetizations m_A, m_B (Appendix I) tend to zero continuously as the temperature is close to the Curie point. So, we observe that, for the values of crystal fields on A-atoms $D_A|J| < -2.2$, the transition temperature may be decreased. However, by using the Oguchi approximation, it has been obtained clear and characteristic behaviors of the molecular-based magnet $AFe^{\mathrm{II}}Fe^{\mathrm{III}}(C_2O_4)_3[A = N(n - C_nH_{2n+1})_4, n = 3-5]$[3, 9,10].

IV. Conclusion

We have investigated the compensation phenomenon of a mixed-spin Blume-Capel Ising ferrimagnetic system composed of $S_i^A = 2$ and $S_j^B = 5/2$, in the application of crystal field .In this work, we have applied OA to the study of a simple cubic lattice to investigate interesting features, one can observe Figs.(4,5,7). Particularly, it has been studied the effect of single-ion anisotropy ,i.e., the crystal field on an existence of compensation temperature. So, our results predict the possibility of many compensation points at low temperatures depending on the negative values of crystal fields(Figs.(6,7)). However, as far as we know, up to now no studies have been made concerning the spin compensation phenomenon of the mixed spin-2 and spin-5/2 Blume-Capel Ising model on the basis of OA. Finally, we can conclude that the crystal field plays a relevant role in the existence of the compensation temperature and it is useful to note that the approximation presented can be used to obtain important results for three-dimensional lattices. It is worth to note that we found unusual behaviours will stimulate experimental and theoretical works on the system which is considered.

Appendix I

By using the Oguchi Approximation, the sublattice magnetizations of the mixed-spin Blume-Capel Ising systems are given:

mA=(2(a1sinh(g1)+b1sinh(g2)+b2sinh(g3)+c1sinh(g4)+c2sinh(g5))+(exp(-3βDA))(a2sinh(h1) -a3sinh(h2)+b3sinh(h3)-b4sinh(h4)+c3sinh(h5)+c4sinh(h6))) / (a1cosh(g1)+exp(-5βJ)+b1cosh(g2)+b2cosh(g3)+c1cosh(g4)+c2cosh(g5)+(exp(-3βDA))(a2cosh(h1) +a3cosh(h2)+b3cosh(h3)+b4cosh(h4)+c3cosh(h5)+c4cosh(h6))+(exp(-4βJDA))(cosh(h7)+cosh(h8)+cosh(h9))) ,

mB=(0.5)(5(a1sinh(x1)+a2sinh(x2)+a3sinh(x3)+sinh(x4))+(3exp(-4βDB))(b1sinh(y1)-b2sinh(y2)+b3sinh(y3)+b4sinh(y4)+sinh(y5))+(exp(-6βDB))(c1sinh(z1)-c2sinh(z2)+c3sinh(z3) -4sinh(z4)+sinh(z5))) / (a1cosh(x1)+exp(-5βJ)+a2cosh(x2)+a3cosh(x3)+cosh(x4)+(exp(-4βDB))(b1cosh(y1)+b2cosh(y2)+b3cosh(y3)+b4cosh(y4)+cosh(y5)) +(exp(-6βDB))(c1cosh(z1)+c2cosh(z2)+c3cosh(z3)+c4cosh(z4)+cosh(z5))) ,

where,

x1=5βJ(z-1)mA ; x2=3.75βJ(z-1)mA ; x3=1.25βJ(z-1)mA ; x4=2.5βJ(z-1)mA ; y1=4βJ(z-1)mA ; y2=βJ(z-1)mA ; y3=2.75βJ(z-1)mA ; y4=0.25βJ(z-1)mA ;
y5=1.5βJ(z-1)mA ; z1=3βJ(z-1)mA ; z2=2βJ(z-1)mA ; z3=1.75βJ(z-1)mA ;
z4=0.75βJ(z-1)mA ; z5=0.5βJ(z-1)mA ; x11=5.0βJ(z-1)mA ; x22=3.75βJ(z-1)mA ; x33=1.25βJ(z-1)mA ; x44=2.5βJ(z-1)mA ; y11=4.0βJ(z-1)mA ; y22=βJ(z-1)mA ;
y33=2.75βJ(z-1)mA ; y44=0.25βJ(z-1)mA ; y55=1.5βJ(z-1)mA ; z11=3βJ(z-1)mA ;
z22=2βJ(z-1)mA ; z33=1.75βJ(z-1)mA ; z44=0.75βJ(z-1)mA ; z55=0.5βJ(z-1)mA ;
g1=4βJ(z-1)mB ; g2=3.2βJ(z-1)mB ; g3=0.8βJ(z-1)mB ; g4=2.4βJ(z-1)mB ;
g5=1.6βJ(z-1)mB ; h1=3βJ(z-1)mB ; h2=βJ(z-1)mB ; h3=2.2βJ(z-1)mB ;
h4=0.2βJ(z-1)mB ; h5=1.4βJ(z-1)mB ; h6=0.6βJ(z-1)mB ; h7=2βJ(z-1)mB ;
h8=1.2βJ(z-1)mB ; h9=0.4βJ(z-1)mB ; a1=exp(5βJ) ; a2=exp(2.5βJ) ;
a3=exp(-2.5βJ) ; b1=exp(3βJ) ; b2=exp(-3βJ) ; b3=exp(1.5βJ) ; b4=exp(-1.5βJ) ;
c1=exp(βJ) ; c2=exp(-βJ) ; c3=exp(0.5βJ) ; c4=exp(-0.5βJ) ; d1=(2βJ(z-1)mB+2.5βJ(z-1)mA) ;

d2=(2βJ(z-1)mB-2.5βJ(z-1)mA) ; d3=(2βJ(z-1)mB+1.5βJ(z-1)mA) ; d4=(2βJ(z-1)mB-1.5βJ(z-1)mA) ; d5=(2βJ(z-1)mB+0.5βJ(z-1)mA) ; d6=(2βJ(z-1)mB-0.5βJ(z-1)mA) ; d7=(βJ(z-1)mB+2.5βJ(z-1)mA) ;
d8=(βJ(z-1)mB-2.5βJ(z-1)mA) ; d9=(βJ(z-1)mB+1.5βJ(z-1)mA) ; d10=(βJ(z-1)mB-1.5βJ(z-1)mA) ;
d11=(βJ(z-1)mB+0.5βJ(z-1)mA) ; d12=(βJ(z-1)mB-0.5βJ(z-1)mA) ;
d13=(2.5βJ(z-1)mA) ; d14=(1.5βJ(z-1)mA) ; d15=(0.5βJ(z-1)mA) ; k1=β (5J+4DA+6.25DB) ;
k2=β (-5J+4DA+6.25DB) ; k3=β (3J+4DA+2.25DB) ; k4=β (-3J+4DA+2.25DB) ;
k5=β (J+4DA+0.25DB) ; k6=β (-J+4DA+0.25DB) ; k7=β (2.5J+DA+6.25DB) ;
k8=β (-2.5J+DA+6.25DB) ; k9=β (1.5J+DA+2.25DB) ; k10=β (-1.5J+DA+2.25DB) ; k11=β (0.5J+DA+0.25DB) ; k12=β (-0.5J+DA+0.25DB) ; k13=(6.25βDB) ;
k14=(2.25βDB) ; k15=(0.25βDB) ;

The free energy of the model is defined as :

$$F \equiv -k_B T \ln Z ,$$

that,

Z=2(exp(k1)cosh(d1)+exp(k2)cosh(d2)+exp(k3)cosh(d3)+exp(k4)cosh(d4) +exp(k5)cosh(d5)+exp(k6)cosh(d6)+exp(k7)cosh(d7)+exp(k8)cosh(d8)+exp(k9)cosh(d9)+exp(k10)cosh(d10)+exp(k11)cosh(d11)+exp(k12)exp(d12)+exp(k13)cosh(d13)+exp(k14)cosh(d14)+exp(k15)cosh(d15))

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