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Spin compensation temperatures in the Oguchi approximation of the mixed $spin-3/2$ and $spin-5/2$ Isingferrimagnet

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Abstract

Using the Oguchi lattice, mixed $spin-3/2$ and $spin-5/2$ Isingmodel with different anisotropies has been tested. The Helmholtzfree energy of a mixed spin Blume-Capel ferrimagnet from Oguchi method of the Hamiltonian is calculated. By reducing the free energy, the equilibrium magnetizations and compensation pointsare evaluated. Explicitly, the influence of magnetic crystalline anisotropies, on the compensation phenomenon, acting on sublattice atoms A and Bhas been investigated, respectively. The crystalline magnetic anisotropy dependence of Curie temperaturehas been discussed as well. The results of this model has predict that the existence of many(two or three) compensation points in the orderedsystem with $z=6$ is strongly dependent on the crystalline magnetic anisotropy D_B.

Keywords: Mixed-spin Ising model; Oguchi approximation; Single-ion anisotropy;Compensation temperature; Phase transition.

I.Introduction

Recently, manyresearchers directed their efforts to the field offerrimagnetic materials, particularlybecause of their wide scope of technological applications [1,2].

In a ferrimagnetic material two inequivalent moments, alignedantiferromagnetically, which gives a zero value of spontaneous magnetizationbelow its Curiepoint[3]. So, a certainpoint, which is called compensation temperature, (T_K) can be observed at a temperature below the critical one (T_c), where the sublatticemagnetic spins cancel exactly each other[4-8]. ErhanAlbayrak studied the critical phenomena of the mixed $spin-3/2$ and $spin-5/2$ Blume–Capel Isingferrimagnetic system on $z=3,4,5$ and 6 by the use of recursion relations[9].Our model is developed and examined within the structure of the Oguchi approach(OA) through reducing the Helmholtz free energy. The magnetic characteristics of the mixed-spin model,havebeen investigated numerically by the using ofMonte Carlo simulations [10,11], to clarify the characteristic magnetic features in a many types of crystal structures.The considered system has been studied previously by the use of mean field theory with neglecting the correlation between atoms [12]. An experimental study has been done on the ferrimagnetic compound $Cs_2Mn^{II}[V^{II}(CN)_6]$, that crystallizes in face centered cubic lattice, prepared by the addition ofmanganese $(II)(S_B=5/2)$ triflate to aqueous solutions of thehexacyanovanadate $(II)(S_A=3/2)$ ion at $0C^o$ [13]. The framework features of the current model are given by finding sublattice magnetizations ordering of the system so the comprehensive analysis of the phase diagrams must be done numerically. An approximate solution of a ferrimagnetic mixed spins Ising model with different crystal fields are obtained for the mixed $spin-3/2$ and $spin-5/2$. As far as we know anIsing model of the mixed-spin ferrimagnet on $z=6$ in which the two mixing sublattices have spins three-half ($\pm1/2,\pm3/2$) and spins five-half($\pm1/2,\pm3/2,\pm5/2$), has not been examined within Oguchi approach(OA).So, instead of using the decoupling approximation, we have introduced the concept of correlation behavior to comprehend the corporative effects exhibited by such systems.A number of experimental efforts in the field of molecular-based magnetic materials and biomaterials have been stimulated and magnetic properties have become an important focus of scientific interest [14,15]. Important advances have been made in the synthesis of two and three-dimensional ferrimagnets.The outline of this work is distributed as follows: in section II we will develop the Hamiltonian of the theorized system and establish our formulas of the sublattice magnetic ordering and free energy. Section III deals with the results that we have obtained, and section IV is the conclusion of this publication.

II. Theory

The Ising model of the mixed-spin ferrimagnet, consists of 3D sublattices S_i and S_j with spins $S_i^A = \pm 1/2, \pm 3/2$ and $S_j^B = \pm 1/2, \pm 3/2, \pm 5/2$ respectively. In this publication, the system is describedusing the Oguchimethodas follows [16], 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,

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

where, $J < 0$. and J is the exchange interaction parameter between lattice sites i and j. z is the coordination number spins, the sublattice magnetic ordering 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 $m_B = < S_j^B >$. D_A, D_B are the crystalline magnetic anisotropies, i.e., the crystal field effects, acting on the $spin-3/2$ and $spin-5/2$ .Let's suppose that the Hamiltonian (1) can be divided into two parts, that is H_A which is related to A atoms and H_B which is related to B atoms.

The identification of the partition function(Z) allowsto demonstrate the relations of thermodynamic quantities. Then, the Helmholtz free energy of the model is determined as[17],

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

where F is the Helmholtzfree energy of *Hamiltonian* given by relation (1), $\beta = \frac{1}{K_B T}$ is Lagrange coefficient, k_B is Boltzmann constant and T is the absolute temperature.So, thesublattice magnetic ordering per site is obtained by reducing theHelmholtzfree energy (Eq.2).It is importantto mention that in ferrimagnetic case the signs of sublattice magnetic orderings are different, and there might be a compensation points at which the total longitudinal magnetic ordersper lattice site equals to zero [18], that:

is equal to zero. $M_T = \frac{1}{2}(m_A + m_B)$

The sublattice magnetization can be predicted by using Maxwell Boltzmann statistics as follows:

$$m_A = \frac{\sum_{S_i} S_i e^{-\beta H_A}}{Z_A} \quad (3a) \qquad m_B = \frac{\sum_{S_j} S_j e^{-\beta H_B}}{Z_B} \quad (3b)$$

Where, $Z_A = \sum_{S_I} e^{-\beta H_A}$ and, $Z_B = \sum_{S_j} e^{-\beta H_B}$.

The compensation points can be calculated from the intersection points between the magnetization curves of m_A and m_B[19].

where $|m_A(T_k)| = |m_B(T_k)|$, i.e.sign $m_A(T_k)$ =-sign $m_B(T_k)$

so that $M_T = |m_A| - |m_B| = 0$, at T_k, and by using Eqs. (1), (2), (3a) the magnetization for the lattice A is:

$$m_A = \frac{1}{2}\begin{pmatrix} 3[a_1\sinh(g_1)+b_1\sinh(g_2)+b_2\sinh(g_3)+b_3\sinh(g_4)+ \\ b_4\sinh(g_5)]+e^{-2\beta D_A}[a_2\sinh(h_1)-a_3\sinh(h_2)+b_3\sinh(h_3) \\ +b4\sinh(h_4)+c_1\sinh(h_5)+c_2\sinh(h_6)] \end{pmatrix} /$$

$$\begin{pmatrix} a_1\cosh(g_1)+e^{-\frac{15}{4}t}+b_1\cosh(g_2)+b_2\cosh(g_3)+b_3\cosh(g_4)+ \\ b_4\cosh(g_5)+e^{-2\beta D_A}[a_2\cosh(h_1)+a_3\cosh(h_2)+b_3\cosh(h_3)+ \\ b_4\cosh(h_4)+c_1\cosh(h_5)+c_2\cosh(h_6)] \end{pmatrix} \quad (4)$$

where,

$$\left.\begin{aligned} & g_1 = 3(z-1)tm_B \;;\quad g_2 = 2.4(z-1)tm_B \;;\quad g_3 = 0.6(z-1)tm_B \\ & g_4 = 1.8(z-1)tm_B ;\quad g_5 = 1.2(z-1)tm_B \;;\quad h_1 = 2(z-1)tm_B \\ & h_2 = (z-1)tm_B \;;\quad h_3 = 1.4(z-1)tm_B \;;\quad h_4 = 0.4(z-1)tm_B \\ & h_5 = 0.8(z-1)tm_B ;\quad h_6 = 0.2(z-1)tm_B . \end{aligned}\right\} \quad (5)$$

and,

$$\left.\begin{aligned} & a_1 = e^{\frac{15}{4}t} \;;\quad a_2 = e^{\frac{5}{4}t} \;;\quad a_3 = e^{-\frac{5}{4}t} \;;\quad b_1 = e^{\frac{9}{4}t} \;;\quad b_2 = e^{-\frac{9}{4}t} \\ & b_3 = e^{\frac{3}{4}t} \;;\quad b_4 = e^{-\frac{3}{4}t} \;;\quad c_1 = e^{\frac{1}{4}t} \;;\quad c_2 = e^{-\frac{1}{4}t} . \end{aligned}\right\} \quad (6)$$

then using Eqs. (1), (2), (3b) to deduce the magnetization formula for lattice B:

$$m_B = \frac{1}{2}\begin{pmatrix} 5[a_1\sinh(x_1)+a_2\sinh(x_2)+a_3\sinh(x_3)]+3e^{-4\beta D_B} \\ [b_1\sinh(y_1)+b_2\sinh(y_2)]+b_3\sinh(y_3)+b_4\sinh(y_4)]+e^{-6\beta D_B} \\ [b_3\sinh(z_1)+b_4\sinh(z_2)+c_1\sinh(z_3)-c_2\sinh(z_4)] \end{pmatrix} /$$

$$\left(\begin{array}{l} a_1\cosh(x_1)+e^{-\frac{15}{4}t}+a_1\cosh(x_2)+a_3\cosh(x_3)+e^{-4\beta D_B} \\ [b_1\cosh(y_1)+b_{24}\cosh(y_2)+b_3\cosh(y_3)+b_4\cosh(y_4)]+e^{-6\beta D_B} \\ [b_3\cosh(z_1)+b_4\cosh(z_2)+c_1\cosh(z_3)+c_2\cosh(z_4)] \end{array}\right) \quad (7)$$

where,

$$\left.\begin{array}{l} x_1=5(z-1)m_At\ ;\ x_2=3.3(z-1)m_At\ ;\ x_3=1.6(z-1)m_At \\ y_1=4(z-1)m_At\ ;\ y_2=(z-1)m_At\ ;\ y_3=2.3(z-1)m_At\ ;\ y_4=0.6(z-1)m_At \\ z_1=3(z-1)m_At\ ;\ z_2=2(z-1)m_At\ ;\ z_3=1.3(z-1)m_At\ ;\ z_4=0.3(z-1)m_At \end{array}\right\} \quad (8)$$

and, $t=\beta J$, where J is the exchange interaction

III. Results and Discussion

It is interesting to examine the magnetic characteristics(the phase diagrams) of the system. It is clear to notice that the Curie(or critical) temperature is dependent of crystal field effects $D_A/|J|$, $D_B/|J|$ effecting on the sublattices A and B atoms, respectively. All of our results have been establishedwhile assuming thattheexternal magnetic field equals zero.

First let's discuss the obtained results by Oguchi method and compare themto mean field theory[12]. We see from Fig.1(a) the global magnetic ordering ofthe consideredsystem for $D_A/|J|=2.0$ and $D_B/|J|=-0.5$,goes to zero more

rapidly than that of the MFA. This is the reason of coupled effect of Oguchi's pair that is correlated to the remaining of the lattice within effective field (the area between the two curves)[20]. One can observe, Fig.1(b), for the sublattice magnetic orderingat the same values of single-ion anisotropies.

Now we will investigate the Curie point and Order parameter under the effect of different ion anisotropies $D_A/|J|$ and $D_B/|J|$ as shown in Fig.2which displays the total magnetizations versus $K_BT/|J|$. For a fixed value of single-ion anisotropy $D_A/|J|=-0.5$ andunequal values of $D_B/|J|$, it is clear that the critical temperature T_C depends substantially on the crystal fields where the area under the curve is the ordered phase withthe negative values of $D_B/|J|$, comparing with that of the positive ones $D_B/|J|$, so the critical pointsfor $D_B/|J|=-1.5,1.5$ are $T_C=7.6K^O$, and $T_C=13.5K^O$, respectively.

Now, let's examine the compensation behavior of the Ising model mixed $spin-3/2$ and $spin-5/2$ Blume-Capel, for $z=6$ with different crystal anisotropies through which we consider the distinctive magnetic characteristics of the system in the absence of the external magnetic field. Fig.3stands for the overallorder parameter versus the absolute temperature, for various values of $D/|J|$. We can recognize that there is a reaction of the system to producethree compensation points in a particular range of negative values of magnetic crystalline anisotropy, namely, $D_A/|J|=2.1, D_B/|J|=-2.0$. Whereas one can spot in the Fig.(4) the system compensates at a certain value of temperature which vanishes the global magnetization. So,the behaviors can be acquired by solving the related equations of m_A and m_B numerically, depending on certain values of crystalline magnetic fields of D_A when $D_B/|J=|-2.5$.

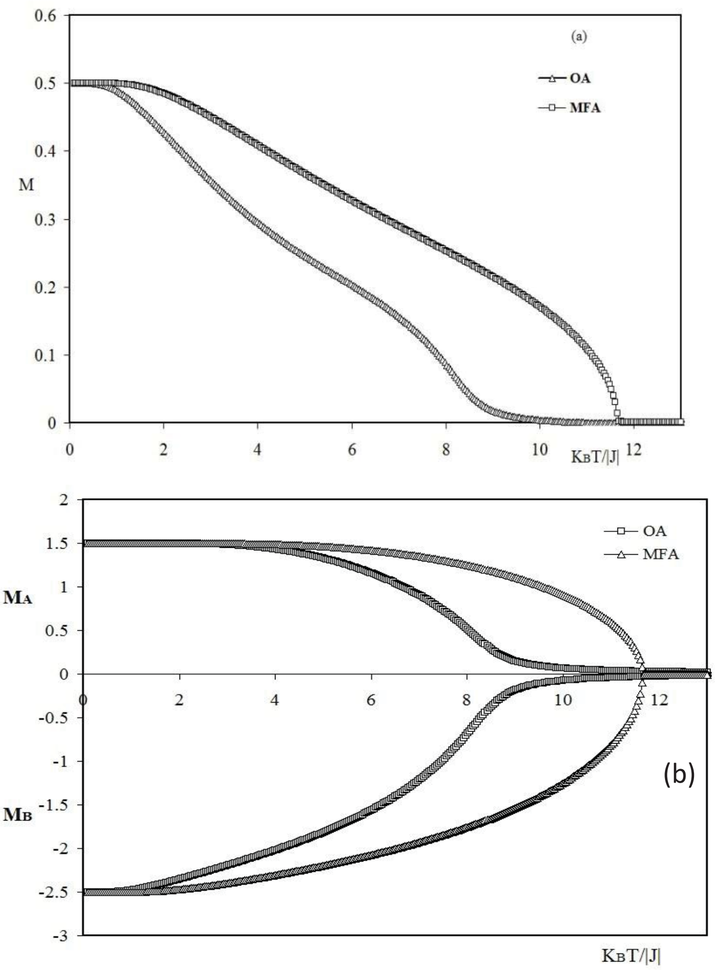

Fig.1 comparison between Oguchi approximation (OA) and Mean-Field approximation (MFA) at $D_A/|J|=2$ and $D_B/|J|=-0.5$ (a) for total magnetization, (b) for sublattices magnetization.

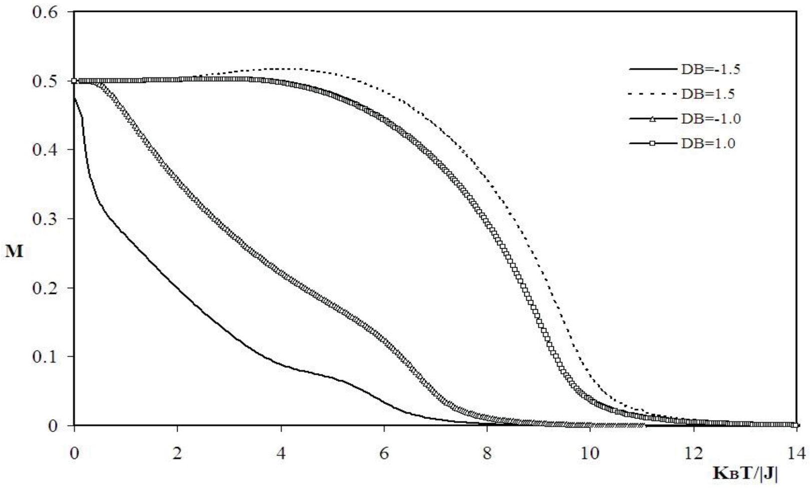

Fig.2. The temperature dependences of the global magnetization M for the mixed-spin ferrimagnetic system with z=6 (number of neighbors), when the value of $D_A/|J|$=-0.5.

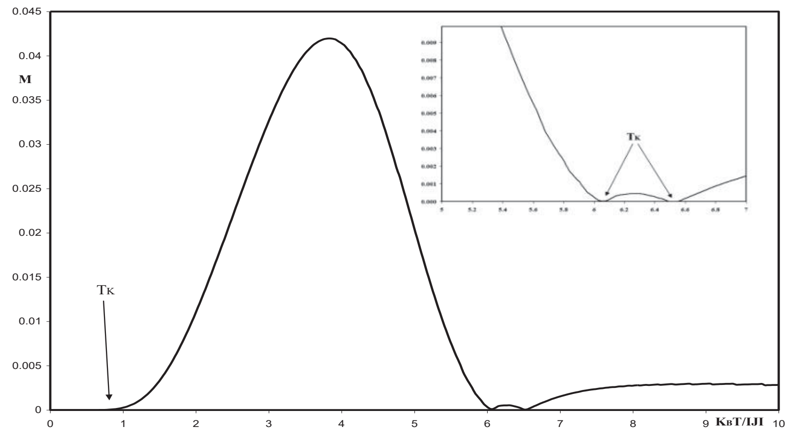

Fig.3. The temperature dependences of the overall magnetization M for the mixed-spin ferrimagnetic system with the coordination number z=6, when the values of $D_A/|J|$=2.1, $D_B/|J|$=-2.0.

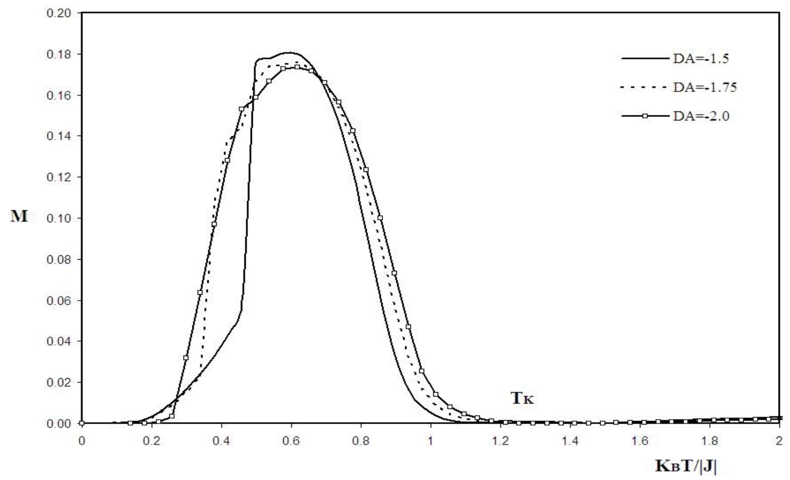

Fig.4. thermal variation of the global magnetization M for the mixed spin ferrimagnetic system with z=6and fixed value of $D_B/|J|$=-2.5.

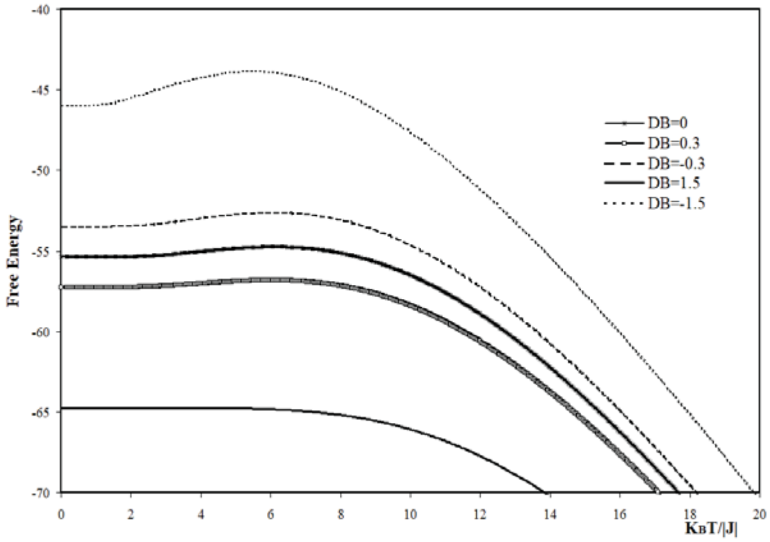

Fig.5. The temperature dependences of Helmholtzfree energy F for the mixed-spinIsingferrimagnetic model with z=6, for different values of $D_B/|J|$, when $D_A/|J|$=-0.5.

On the other hand, the contribution of Helmholtz free energy to the phase steadiness of the mixed spin ferrimagneticIsingmodel have also been taking into consideration. Free energy versus $K_B T/|J|$ has been estimated according to Eq.(2), as shown in Fig.4. For the description of the Helmholtzfree energy of the or antiferromagnetic phase (at the point of compensation) and paramagnetic state (at Curie temperature), one can deduce that the free energy curve has an flexure that it indicates a discontinuous behaviourand at Curie point the Helmholtzfree energy of the system is continuous. The results shown in Fig.5 have a consistentpatternwiththosederivedfromFig.2.

IV. Conclusion

We have examined the existence of compensation phenomena in a ferromagnetic Blume–Capel Ising system of mixed $spin-3/2$ and $spin-5/2$ using OA on a $z=6$ latticewith no external magnetic induction. The phase diagrams of the system with unequal crystal fieldshave been perceivedby working out the main expressions numerically. So, the overall magnetization curves have revealed some outstanding features (many compensation points). We can distinguish our results from thoseacquired in the mean-field approach[12], in which the model didn't show any compensation temperatures.Nevertheless, wenow have awareness that there is no response of the system to yield a compensation point in the range of positive values of crystal field effects, in contrast to negative ones influencing the existence and magnitude of the compensation points, as shown in Figs.(3,4), respectively.

Besides, the assistance of Helmholtz free energy to the phase steadiness of the mixed spin ferrimagnet which is considered has also been surveyed. Finally, we expect that this work may haveboost and illustrate the characteristic features, for the appearance of a compensation behavior at low temperatures, in a different classes of molecular-based ferrimagnets and Biological models.

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