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MAGNETIC PROPERTIES AND FREE ENERGY OF A MIXED SPIN-1/2 AND SPIN-1 FERRIMAGNET

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ABSTRACT

The magnetic behaviours of a mixed Blume-Capel Ising ferrimagnetic system on a square lattice having spins $\sigma_i^A = \pm\frac{1}{2}$ and spins $\sigma_j^B = 0,\pm 1$, in the absence and presence of an external magnetic field, are investigated, respectively. Our results which are examined have interesting features depending on higher positive values of anisotropy field. The longitudinal magnetic fields dependence of the spin compensation temperature is the essential substance of research. It is worth to note that in this model, the contribution of magnetic free energy to the thermodynamic stability of the mixed spin ferrimagnet with first nearest neighbour interaction is indicated.

KEYWORDS: Mixed Spin, Blume-Capel Model, Ferrimagnet, Magnetic Field, Gibbs Free Energy, Compensation Temperature

INTRODUCTION

During the last years a lot of efforts has been directed to the study of critical phenomena in mixed-spin Ising systems consisting of spin-1/2 and spin-S atoms with $S > 1/2$. These systems are well adapted to study a certain type of ferrimagnetism, namely molecular-based magnetic materials which are of great interest because of its interesting and possibly useful properties for technological applications and academic research[1,2,3]. Ferrimagnets are materials where ions on different sublattices have opposing magnetic moments and show paramagnetic behaviour above transition temperature (T_c)[4,5,6]. T.Kaneyoshi[7], has investigated a mixed Ising ferrimagnetic system consisting of spin-1/2 and spin-1 and found a compensation point induced by the different transverse fields. The compensation phenomenon of the mixed spin ferrimagnetic system on a square lattice in the presence of an oscillating magnetic field has been studied by G. Buendia[8]. On the other hand, J.Oitmaa et al[9] introduced mixed-spin models on a decorated simple cubic lattice showing a compensation behaviour. The authors[10] found, in a series study of a mixed-spin model, in the absence of an external magnetic field, that the model with nearest neighbor interactions only, does not appear to have a ferrimagnetic compensation point.

Other researchers[3,4], in this respect, observed that the effect of next-nearest-neighbour interaction between the spin sites on the lattice possibly leads to a compensation phenomenon. The single-ion anisotropy and external fields may cause a compensation temperature, as well[6,11].

It is worth to note that several theoretical investigations have recently been reported concerning a mixed-spin model with different longitudinal fields[6,12]. However, in this research, we have interested to study a ferrimagnetic mixed spin $\sigma_i^A = \frac{1}{2}$ and spin $\sigma_j^B = 1$ Blume-Capel Ising model. The work includes, in Section 2, a formulation of the model and its mean field solution. It has been calculated the magnetic Gibbs free energy of the model, as well. Finally, we discuss, in Section 3, the possibility of multicompensation points, for various values of the anisotropies and longitudinal fields, respectively, at low temperatures. Besides, it has been examined the free energy behaviour of the mixed system.

Theory

The model which is considered consists of two interpenetrating sublattices. One sublattice has spins (σ_i^A) that can take two values $(\pm\frac{1}{2})$, the other sublattice has spins (σ_j^B) that can take three values $(0,\pm1)$. Each (σ_i^A) spin has only (σ_j^B) spins as nearest neighbors and vice versa. The Hamiltonian of the mixed-spin Blume–Capel Ising ferrimagnetic system, is given by [13]:

$$H = -J\sum_{i,j}\sigma_i{}^A\sigma_j{}^B - D\sum_j(\sigma_j{}^B)^2 \quad (1)$$

where J is the exchange interaction parameter$(J<0)$, D is the crystal field acting on B-atoms. The system is described, in the presence of an external magnetic field, by the following Hamiltonian[14],

$$H = -J\sum_{i,j}\sigma_i{}^A\sigma_j{}^B - D\sum_j(\sigma_j{}^B)^2 - h\sum_{i,j}(\sigma_i^A + \sigma_j^B) \quad (2)$$

Gibbs free energy of the system is obtained from a mean field calculation of the Hamiltonian based on the Bogoliubov inequality [5,15]:

$$G \le G_0 + \langle H - H_0\rangle_0 \quad (3)$$

where G is the free energy of H given by relation (2), that:

$$G = -k_B T\ln Z\,;\, Z = \sum_{i,j} e^{-\beta H} \quad (4)$$

G_0 is the free energy of a paramagnetic phase and H_0 a trial Hamiltonian depending on variational parameters, that:

$$G_0 = -k_B T \ln Z_0 \,;\, Z_0 = \sum_{i,j} e^{-\beta H_0} \qquad (5)$$

Z, Z_0 are the true partition function and trial one respectively.

In this research we consider one of the possible choices of H_0, namely:

$$H_0 = -\lambda_A \sum_i \sigma_i^A - \sum_j [\lambda_B \sigma_j^B + D(\sigma_j^B)^2] + h\sum_{i,j} (\sigma_i^A + \sigma_j^B) \qquad (6)$$

where λ_A and λ_B are the two variational parameters related to the two different spins σ_i^A and σ_j^B respectively.

By minimizing the right hand of Eq.(3) with respect to variational parameters, we obtain the approximated free energy, that:

$$g = \frac{G}{N} = -\frac{1}{2\beta}[\ln(2\cosh\frac{1}{2}(\beta\lambda_A + h^L)) + \ln(2e^{\beta D}\cosh(\beta\lambda_B + h^L) + 1)] + \frac{1}{2}[-zJm_A m_B + \lambda_A m_A + \lambda_B m_B] \qquad (7)$$

where N is the total number of sites of lattice. Minimizing this expression with respect to λ_A, λ_B we obtain,

$$\lambda_A = Jzm_B \,, \quad \lambda_B = Jzm_A \,, \qquad (8)$$

with,

$$m_A = \frac{1}{2}\tanh\frac{1}{2}(\beta\lambda_A + h^L) \qquad (9)$$

$$m_B = \frac{2\sinh(\beta\lambda_B + h^L)}{2\cosh(\beta\lambda_B + h^L) + e^{-\beta D}} \qquad (10)$$

where $h^L = \beta h$, $\beta = \dfrac{1}{K_B T}$, z is the coordination number of the lattice.

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[3],

$$M = \frac{1}{2}(m_A + m_B)\,, \qquad (11)$$

is equal to zero.

Results and Discussion

At zero temperature, we find two phases with different values of (m_A, m_B, μ), namely, the ordered ferrimagnetic phase $O = \{(1, -\frac{1}{2}), or(-1, \frac{1}{2})\}$ as well, and disordered phase $D = (0, \frac{1}{2}), or(0, -\frac{1}{2})$, where the parameter μ is defined by:

$$\mu = \left\langle (\sigma_j^B)^2 \right\rangle \tag{12}$$

In this research, we examine the spin compensation temperature of a mixed spin-1/2 and spin-1 Blume-Capel Ising ferrimagnetic model, for a square lattice. Now, let us study the phase diagram of the mixed spin ferrimagnetic system with different crystal fields through which we consider the characteristic magnetic properties of the system under the influence of different longitudinal fields.

Fig.1 stands for the total magnetization versus the absolute temperature, in the absence of an external magnetic field, for different values of $D/|J|$. One can see that there is a response of the system for induction of one compensation temperature in the range of negative values of magnetic anisotropy, namely, $D/|J| = -1.85, -1.90, -1.95$. The results shown in the Figures(2,3) are consistent with those derived from Fig.1. Whereas one can observe in the Fig.4, the system doesn't exhibit any compensation points in the thermal variation of the system magnetization, which can be obtained by solving the coupled equations for m_A and m_B numerically, depending on the values of the applied magnetic fields, in the range of values of longitudinal fields, when $h/|J| = -0.1, -0.2, -0.3, -0.4, -0.5$, with a fixed value of anisotropy, for example, $D/|J| = -1.95$, of the sites occupied by B- atoms. It is worth noting that the positive values of $h/|J| = 0.1, 0.2, 0.3, 0.4, 0.5$ when , $D/|J| = -1.95$, make the sublattice magnetizations acting on B-atoms be lost. In the two figures(5,6), we report an interesting feature of compensation temperatures for $D/|J| = 10$, and $D/|J| = 15$ with different positive values of longitudinal fields, when, $h/|J| = 0.3, 0.4, 0.5$ respectively. As shown in the figures, the magnetization shows characteristic thermal variation behaviour that the system may produce three spin compensation points at $T \neq 0$. It is worth mentioning that the increase the value of anisotropy, the increase the compensation temperature. In the region where the system may show multicompensation points, the sublattice magnetization m_A is more ordered than the sublattice magnetization m_B below the compensation temperature. These sublattice magnetizations are still incomplete so there is a residual magnetization in the system[3]. As the values of $h/|J|$ is increased, at certain values of the anisotropies $D/|J|$ acting on the B-atoms, the direction of this residual magnetization may switch. That is to say, due to entropy some spins can flip their directions. Thus, the sublattice magnetization m_B becomes more ordered than the sublattice magnetization m_A for temperatures above the compensation temperature. So there is an intermediate point such that the cancellation is complete $(m_A = -m_B and M = 0)$ [5,6]. 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. Gibbs free energy as a function of temperature has been calculated according to Eq.(3), is shown in Fig.(7). For the description of the free energy of the ferrimagnetic or antiferromagnetic state (at compensation point) and paramagnetic one(at transition temperature), one can observe the free energy curves has 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.(7,8) are consistent with those derived from Figs.(3,5,6).

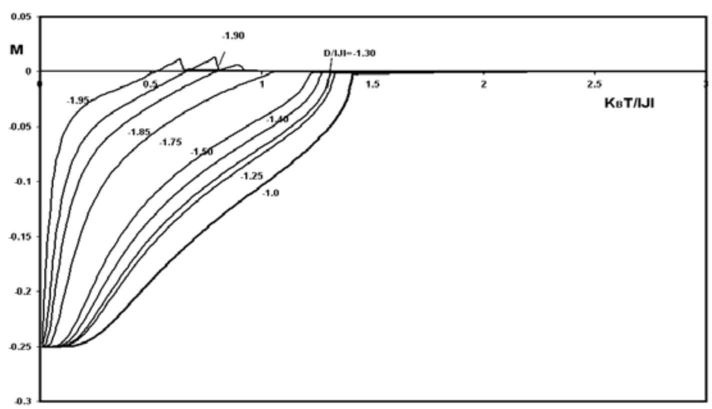

Fig.1. The phase diagram of the mixed spin-$\frac{1}{2}$ and spin-1 ferrimagnetic system for $z = 4$, and different values of $D/|J|$, in the absence of $h/|J|$.

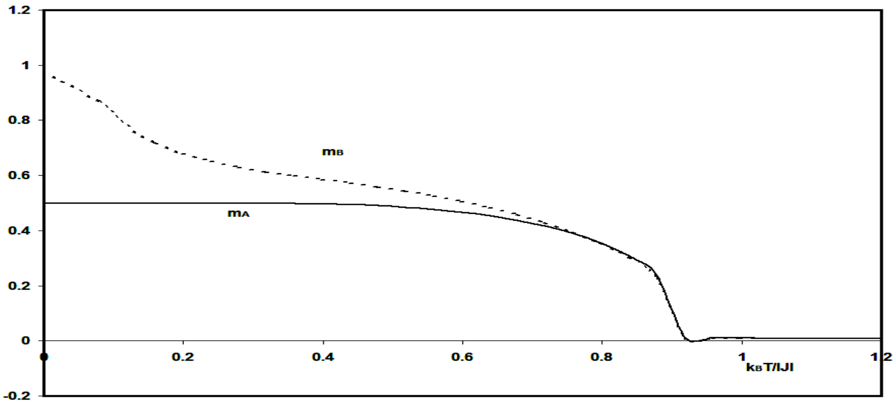

Fig.2. The temperature dependences of the sublattice magnetizations m_A, m_B for the mixed-spin ferrimagnet with the coordination number $z = 4$, at a fixed value of $D/|J| = -1.85$.

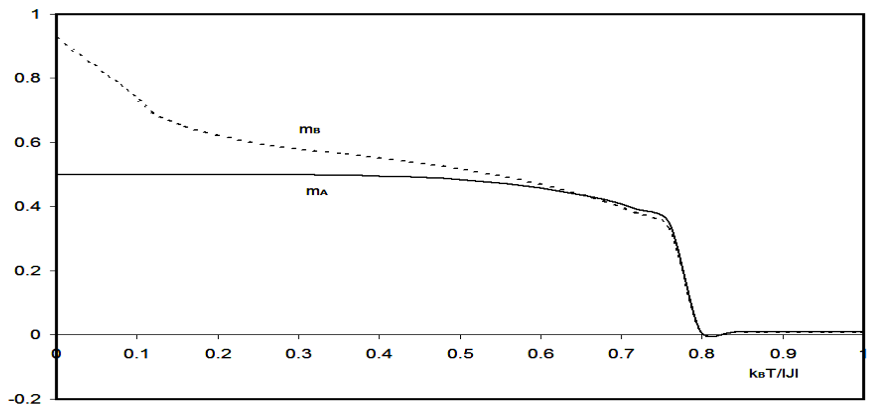

Fig.3. The temperature dependences of the sublattice magnetizations m_A, m_B for the mixed-spin ferrimagnet with the coordination number $z = 4$, at a fixed value of $D/|J| = -1.90$.

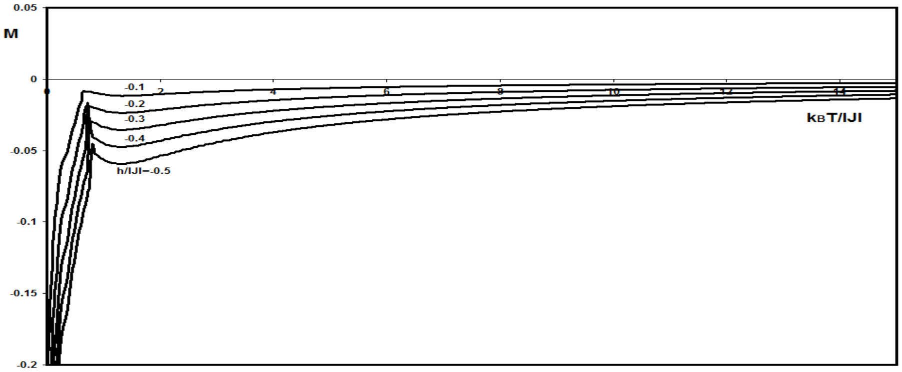

Fig.4. The temperature dependencies of the total magnetization M for the mixed-spin ferrimagnet with the coordination number $z = 4$, for different values of $h/|J|$, at a fixed value of $D/|J| = -1.95$.

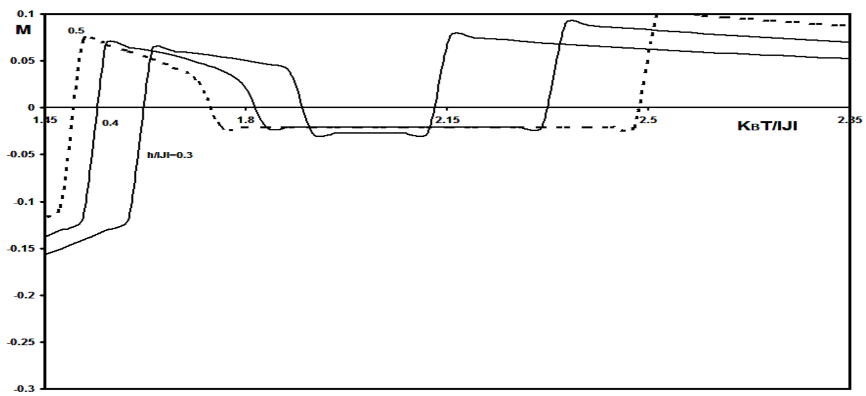

Fig.5. The temperature dependencies of the total magnetization M for the mixed-spin ferrimagnet with the coordination number $z = 4$, for different values of $h/|J|$, at a fixed value of $D/|J| = 10$.

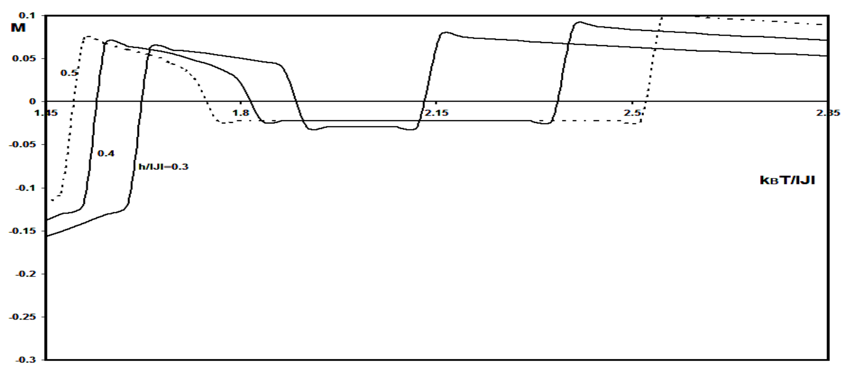

Fig.6. The temperature dependencies of the total magnetization M for the mixed-spin ferrimagnet with the coordination number $z = 4$, for different values of $h/|J|$, at a fixed value of $D/|J| = 15$.

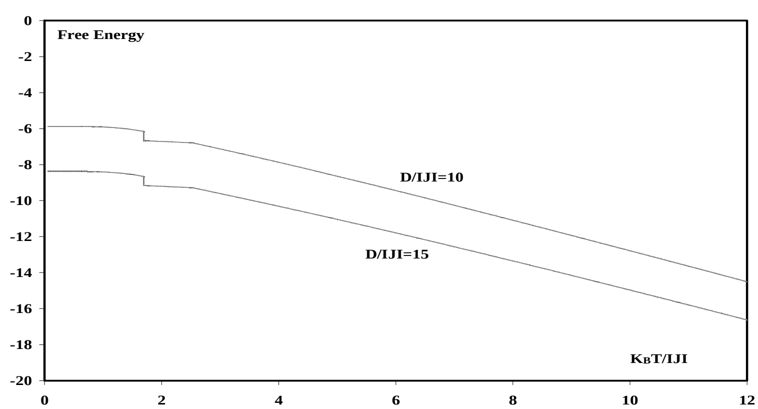

Fig.7. The temperature dependencies of Free Energy G for the mixed-spin ferrimagnet with the coordination number $z = 4$, for $h/|J| = 0.5$, at a fixed value of $D/|J| = 10{,}15$, respectively.

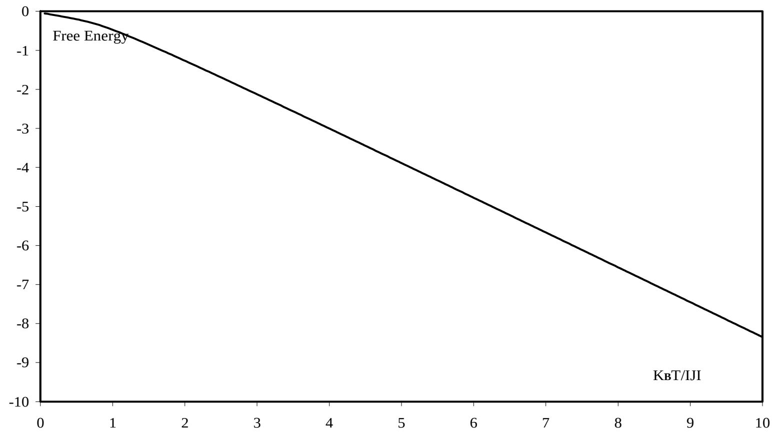

Fig.8. The temperature dependencies of Free Energy G for the mixed-spin ferrimagnet with the coordination number $z = 4$, for $h/|J| = 0.0$, at a fixed value of $D/|J| = -1.90$.

Conclusion

We have studied the compensation phenomenon of a mixed spin-1⁄2 and spin-1 Blume–Capel ferrimagnetic system using MF approximation on a square lattice in the absence and presence of an external magnetic field. The phase diagrams of the system with different anisotropies have been found by solving the general expressions numerically. So, the magnetization curves have exhibited some outstanding characteristics (three compensation points). One can compare our results with those obtained in the mixed spin-1/2 and spin-1 systems[12,16], in which the models show two compensation temperatures, respectively. On the other hand, one can observe that there is no response of the system for induction of a compensation point in the range of negative values of external fields, in contrast to positive ones influencing the existence and location of the compensation points, as shown in the figures(4,5,6), respectively. 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. Finally, we hope that this work may be helpful to support and clarify the characteristic features, for the existence of a compensation point at low temperatures, in a series of molecular-based magnets, when the experimental data of ferrimagnetic materials are analyzed.

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