Ground-State phase diagram of a mixed Ising ferrimagnetic on a square lattice

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Abstract:

The ground-state phase diagram and phase diagrams in the temperature-anisotropy plane of a ferrimagetic mixed spin S^A_j=3/2 and spin S^B_j=5/2 Ising system are investigated by the use of the mean-field theory. Some interesting features are found in the temperature dependences of sublattice magnetizations on a square lattice.

Keywords: Mixed-spin Ising model ;Ferrimagnet; single-ion anisotropy; second-order phase transition.

1. Introduction:

Ferrimagnetisms has been extensively investigated in the past both theoretically and experimentally, since important magnetic materials for technological applications are ferrimagetic [1]. Thus, in recent years, the study of the Ising model with mixed spins of different magnitudes has attracted considerable attention.Most research attention has been directed to the two-sublattice mixed spin system consisting of spin-1/2 and spin-s(s>1/2) with acrystal-field interaction. It has been investigated by a variety of techniques, such as exact , mean-field approximation , and effective-field theory[1-7]O.F Abubrig et al [2] extended the investigations with one constituent having spin-1 and the other constituent having spin -3/2. It have been shown that the magnetic properties of this system has been discovered

experimentally.in($(Ni^{II}_{0.22}Mn^{II}_{0.60}Fe^{II}_{o.18})_{1.5}[Cr^{III}(CN)_6].7.6H_2O$.Therfore it is interesting to investigate a more general mixed-spin Ising model, consisting of spin -3/2 and spin -5/2.

The purpose of this work is to determine the ground-state phase diagram and study sub lattice magnetizations of a mixed spin-3/2 and spin -5/2 ferrimagetic Ising system with a crystal- field interaction on the basis of the standard mean-field theory.

The outline of this work is as follows. briefly presented the basic frame work of the theory based on the Bogoliubov inequality for the Gibbs free energy. The phase diagrams and sublattice magnetizations for various values of the single-ion anisotropies are also discussed Formulation of the model and its mean-field solution :

The model we are going to consider consists of a mixed two magnetic atoms A and B with spins S_i^A=3/2 and S_j^B=5/2 . Then, the Hamiltonian of the system in the Ising model, with H=0 , can be written as[3]:

$$H = -J\sum_{i,j} S_i^A S_j^B - D_A \sum_i (S_i^A)^2 - D_B \sum_j (S_j^B)^2 \text{-----(1)}$$

when $S_i^A = \pm 1/2 , \pm 3/2$, for i belonging to sub lattice A and

$S_j^B = \pm 1/2 , \pm 3/2 , \pm 5/2$, for j belonging to sub lattice B.

D_A , D_B are the anisotropies acting on the nearest-neighbor exchange parameter.

Now , it is used a variational method based on the Bogoliubov inequality for the Gibbs free energy [2,4] :

$$G(H) \leq G(H_0) + \langle H - H_0 \rangle \equiv \phi \text{----(2)}$$

When $G(H)$ is the free energy of Hamiltonian ,$G(H_o)$ is the free energy of a trial Hamiltonian H_o which depends on variational parameters and< ….> denotes a thermal average over the ensemble defined by H_o

We consider in this work one of the simplest possible choices of H_o , namely :

$$H_0 = -\sum_j [\gamma_A S_j^A + D_A (S_j^A)^2] - \sum_j [\gamma_B S_j^B + D_B (S_j^B)^2] \text{......(3)}$$

Where γ_A and γ_B are two variational a parameters related to the two different spins , respectively . Then, the approximated free energy can be obtained by minimizing the right side of equation(2) with respect to variational parameters mentioned above. Thus, the equation(2) can be expressed as:

$$g \equiv \frac{\phi}{N} = -\frac{1}{2\beta}\{lm[2e^{9/4\beta D_A}\cosh(\frac{3}{2}\beta\gamma_A) + 2e^{1/4}\cosh(\frac{1}{2}\beta\gamma_A)] + lm[2e^{25/4\beta D_B}\cosh(\frac{5}{2}\beta\gamma_B) + 2e^{9/4\beta D_B}\cosh(\frac{3}{2}\beta\gamma_B) + 2e^{1/4\beta D_B}\cosh(\frac{1}{2}\beta\gamma_B)]\} + 1/2(-2Jm_A m_B + \gamma_A m_A + \gamma_B m_B) --(4)$$

When N is the total number of sites of lattice . Minimizing this expression with respect to γ_A and γ_B ,we obtain :

$$\gamma_A = ZJm_B \ , \ \gamma_B = ZJm_A \quad \text{--------------(5)}$$

with

$$m_A \equiv \langle S_i^A \rangle_o = \frac{1}{2}\frac{3\sinh(\frac{3}{2}\beta\gamma_A) + e^{-2\beta D_A}\sinh(\frac{1}{2}\beta\gamma_A)}{\cosh(\frac{3}{2}\beta\gamma_A) + e^{-2\beta D_A}\cosh(\frac{1}{2}\beta\gamma_A)} \text{---(6)}$$

$$m_B \equiv \langle S_j^B \rangle_o = \frac{1}{2}\frac{5\sinh(\frac{5}{2}\beta\gamma_B) + 3e^{-4\beta D_B}\sinh(\frac{3}{2}\beta\gamma_B) + e^{-6\beta D_B}\sinh(\frac{1}{2}\beta\gamma_B)}{\cosh(\frac{5}{2}\beta\gamma_B) + e^{-4\beta D_B}\cosh(\frac{3}{2}\beta\gamma_B) + e^{-6\beta D_B}\cosh(\frac{1}{2}\beta\gamma_B)} \text{--(7)}$$

Since the present model is related to the spin -3/2 and spin-5/2 Ising systems for any value of parameters , it undergoes a second-order transition that some features of the phase diagram can be determined analytically. Thus, close to the second-order phase transition from an order state (m_A=o, m_B≠o) to the paramagnetic one(m_A=0 , m_B=o), the

magnetizations m_A and m_B are very small ,so we expand Eqs.[(4),(6),(7)] to obtain a Landau-like expansion [2,5] :

$$g = g_o + a m_A^2 + b m_A^4 + c m_A^6 + o(m_A^8) \quad \text{-------(8)}$$

where g_o is a free energy of the paramagnetic phase and m_A is the order parameter which takes the magnetization value of A-atom at a thermodynamic equilibrium , In this way, the second-order phase transition line is then determined by a=0 and b > 0 . Further , it should also be noted that the critical behavior is the same for both ferromagnetic (J > 0) and ferrimagnetic (J < 0) systems [2,3].

3.Results and discussions :

The ground-state energies determine the phase diagram at zero temperature , one can find six phase with different values of {m_A , m_B , q_A , q_B } , namely the ferrimagnetic phases order as :

O_1≡{3/2 , 5/2 , 9/4 , 25/4} , O_2 ≡ {1/2 , 5/2 , 1/4 , 25/4 }

O_3≡{3/2, 3/2 , 9/4, 9/4 } , O_4≡{1/2 , 3/2 ,1/4 , 9/4}

O_5≡{3/2 , 1/2 , 9/4 , 1/4} , O_6≡{1/2 , 1/2 , 1/4 , 1/4 } .

The are no disordered phases where the parameters q_A and q_B defined by :

$$, \quad q_A = \langle (S_i^A)^2 \rangle \quad , \quad q_B = \langle (S_j^B)^2 \rangle \quad \text{-----------(9)}$$

The corresponding ground-state energies per site for these phases are , respectively ,

$$Uo_1 = -\frac{15Z|J|}{8} - \frac{9D_A}{8} - \frac{25D_B}{8} \quad \text{------------------(10)}$$

$$Uo_2 = -\frac{5Z|J|}{8} - \frac{D_A}{8} - \frac{25D_B}{8} \quad \text{--------------------(11)}$$

$$Uo_3 = -\frac{9Z|J|}{8} - \frac{9D_A}{8} - \frac{9D_B}{8} \quad \text{--------------------(12)}$$

$$Uo_4 = -\frac{3Z|J|}{8} - \frac{D_A}{8} - \frac{9D_B}{8} \quad \text{-----------------------(13)}$$

$$Uo_5 = -\frac{3Z|J|}{8} - \frac{9D_A}{8} - \frac{D_B}{8} \quad \text{----------------------(14)}$$

$$Uo_6 = -\frac{Z|J|}{8} - \frac{D_A}{8} - \frac{D_B}{8} \quad \text{-----------------------(15)}$$

By comparing the energies we determine the phase diagram shown for the system with Z= 4 in Eq .1 .

The second-order phase transition lines are analytically obtained through a Landau free energy expansion in the order parameter , that one is able to evaluate equation (8) , by setting a = 0 . Let us consider the case when 16≤ D_B ≤ - 10 . Fig. (2) shows the phase diagrams in the (D_A , T) plane for various values of D_B ⁄ | J | . We see that a certain type of phase diagram is achieved with second-order transitions at different values of transition temperature , That is to say , phase transitions related to anisotropy continuity showing second-order behavior . Our results could be compared with that of spin – 1/2 and spin – 3/2 system using the effective field theory [6] . Further more , one can see that the values of D_B ≥ 16 , the transition temperature can never be increased ; and for D_B ≤ - 10 , the transition temperature can never be lower . It is worth while to not that the system considered here doesn't exhibit a tricritical point since the behaviour of the curves in Fig.(2) allows to see second-order phase transition only [7,8] . Now , let us discuss the temperature dependence of the sub lattice magnetizations m_A ,m_B by solving the coupled Eqs.(5)-(7) numerically . The results are depicted in Fig.(3)for the system with D_A ⁄ |J| = - 6.0 , when the value of D_B ⁄ | J | is changed from D_B ⁄ | J | = -o.3 to – 1.5 .

As shown in Fig.(3) , the possible ordered phases at T= 0K^o are separated at the critical value D_{BC} of D_B, namely , D_{BC} = -1.0 , when D_B ⁄ | J | > - 1.0 , namely , D_B ⁄ | J | = - 0.66 and D_B ⁄ | J | ≥ - 0.5 , the sub lattice magnetization m_B shows normal thermal-variation behaviour. As D_B ⁄ | J | decreases from D_B = - 0.66 , however ,the temperature dependence of m_B may exhibit a rather rapid decrease from its saturation value at T=0k^o . For a value of D_B in the region – 0.66 < D_B ≤ - 0.6 , the temperature

dependence of m_B may increase from the saturation value with increase in T . The phenomenon is further enhanced when the value of D_B approaches the critical value D_{BC} . In particular , at the critical value and for T = 0 K^o , the saturation value of m_B is m_B = 1.0 , which indicates that in the ground state the configuration of S_j^B in the system consists of the mixed state ; in this state half of the spins on the sub lattice B are equal to 3/2 and the other half are equal to 1/2 .

As noted above , when $D_B / | J | < -1.0$, the spin state of S_j^B is in the $S^B{}_j$ =1/2 state at T=0k^o and hence the saturation magnetization is given by m_B = 0.5 . On the other hand , for all values of D_B the sublattice magnetization m_A may show normal behaviour , even though it is coupled to m_B .

4.Conclusions :

We have applied the mean-field theory to a mixed Ising ferrimagnetic system on a square lattice consisting of spin – 3/2 and spin – 5/2 with different single-ion anisotropies D_A and D_B acting on the spin – 3/2 and spin – 5/2 ,respectively . The ground –state phase diagram are calculated exactly . on the other hand, the phase diagram at low temperature and the sublattice magnetizations of this work have shown some characteristics different from the corresponding mixed spin – 1/2 and spin – 3/2 system . It is interesting to note that in the present system there is no tricritical behaviour. The system investigated here is a fruitful one from both the theoretical and experimental points of view .

The present study will be benefited when the experimental data of ferrimagnetic materials are analyzed.

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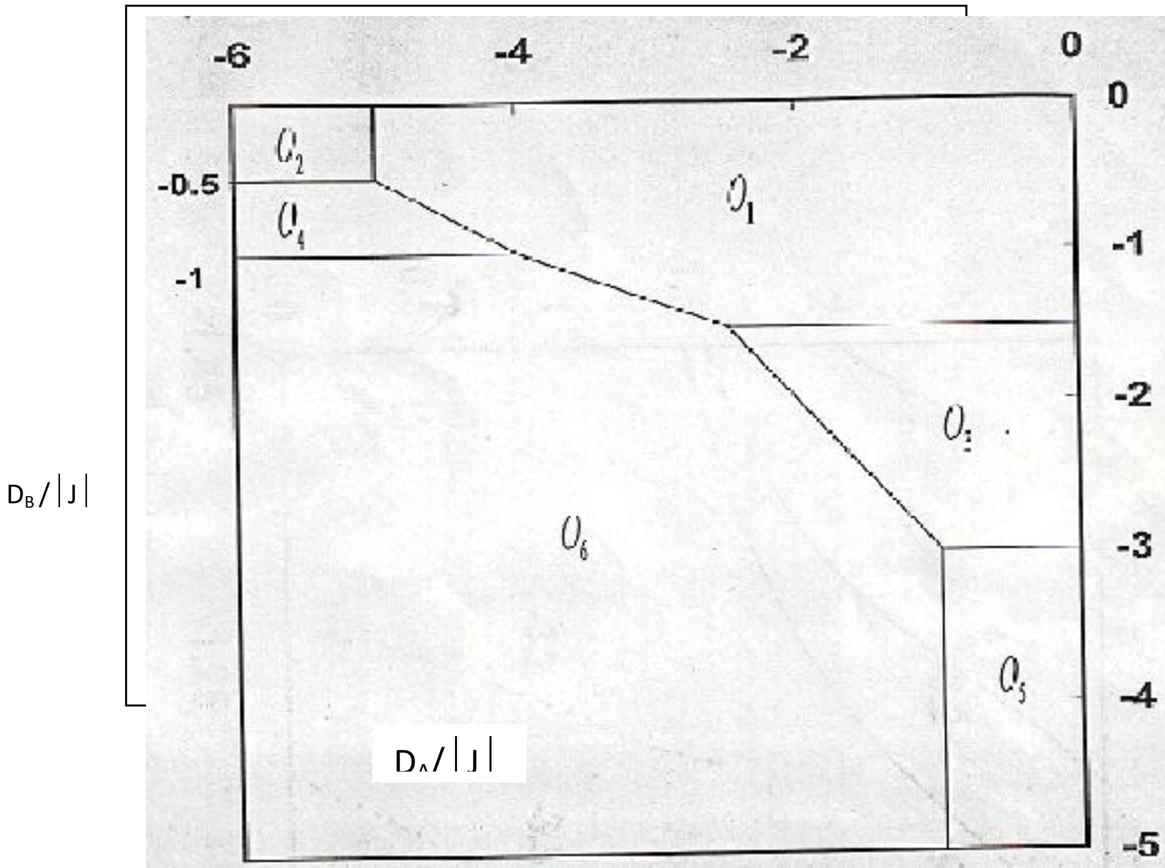

Fig.1.

Ground-statephase diagram of the mixed spin – 3/2 and spin – 5/2

Ising ferrimagnetic system with Z=4 (square lattice)

And different single-ion anisotropies D_A and D_B .

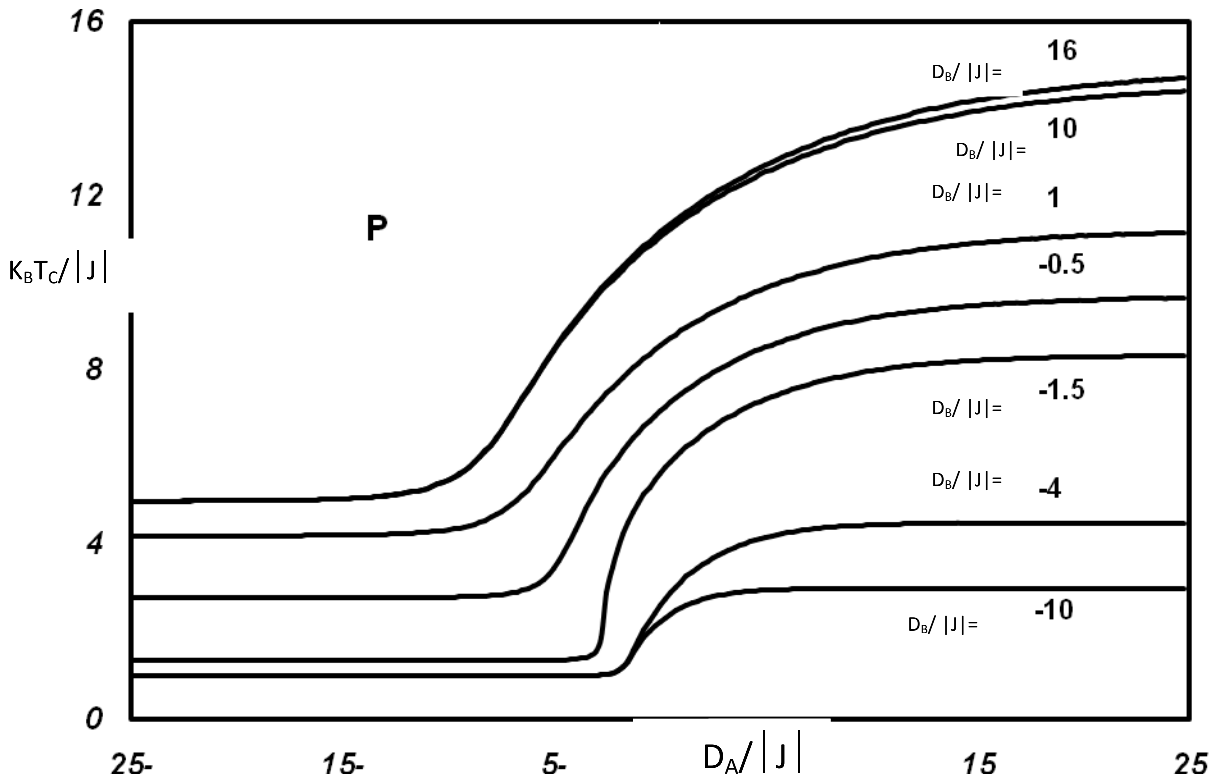

Fig.2

. Phase diagrams in the (D_A , T) plane for the mixed- spin Ising ferrimagnetic system on a square lattice , when the value of D_B is changed .The solid lines indicate second- order phase transition . P is the paramagnetic phase .

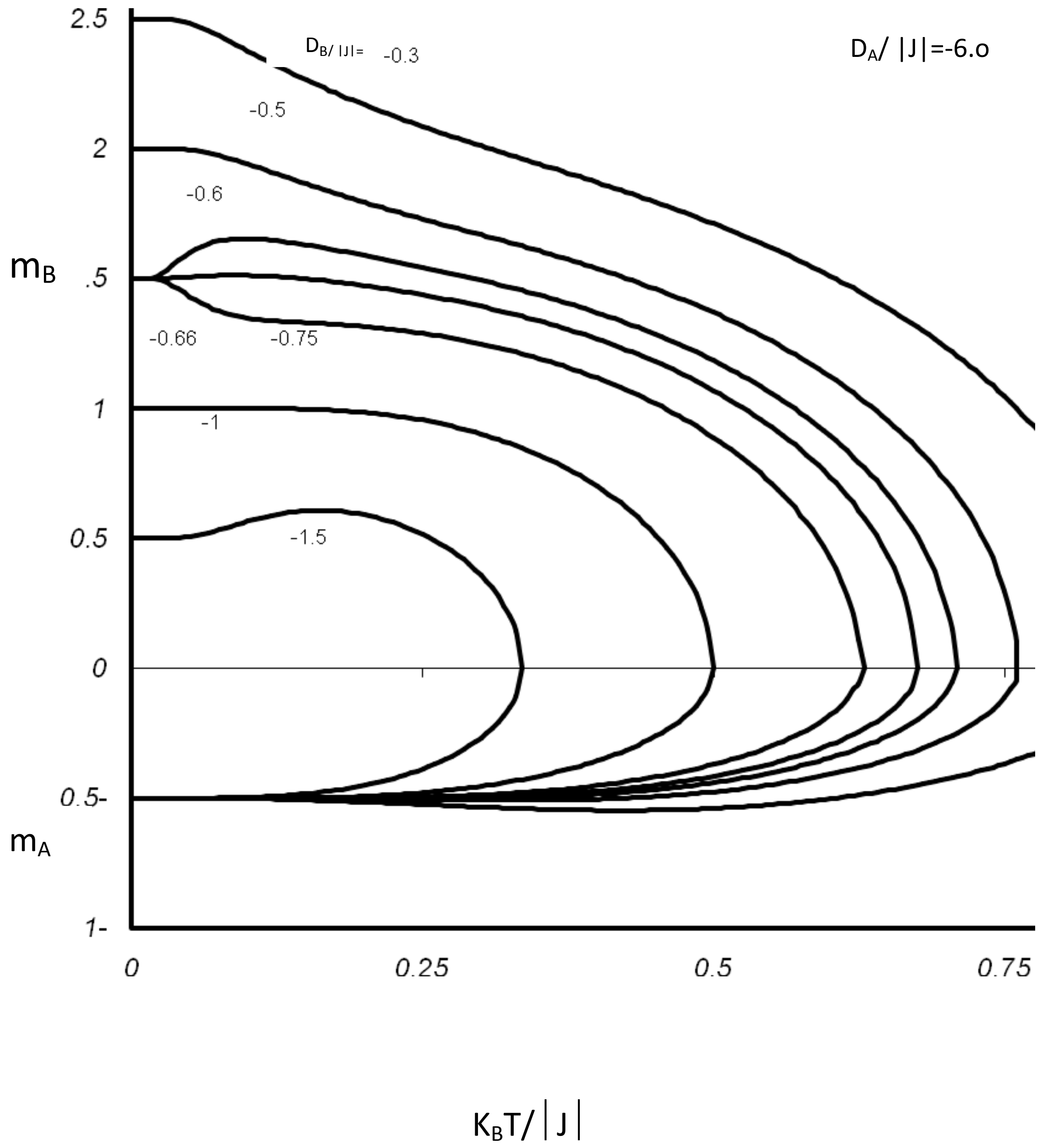

Fig. 3.

The temperature dependences of the sublattice magnetizations m_A , m_B for the mixed – spin Ising ferrimagnetic system with Z= 4 (square lattice), when the value of $D_B / | J |$ is changed , for fixed $D_A / | J | = - 6.0$.

الخلاصة:

مخطط طور الحالة الارضية للمواد الفيرومغناطيسية(لخليط ايزنك) على شبيكة تربيعية

في هذه الدراسة تم البحث في أيجاد المخطط ألطوري للحالة الأرضية وكذلك المخططات الطورية في المستوي(تباين- درجة حرارة) لنظام ايزنك فيريمغناطيسي خليط يتكون من شبيكتين فرعيتين A، B عزومهما المغناطيسية ($S_i^A=3/2$ ، $S_j^B=5/2$) على التوالي ، باستخدام نظرية متوسط المجال . وقد وجدنا بعض الخصائص ذات الاهتمام البحثي عند دراسة العزم المغناطيسي المتوسط للنظام المذكور على شبيكة رباعية دالة لدرجة الحرارة المطلقة .