Mean-field Solution of the mixed spin-1 and spin-5/2 Ising system with different single-ion anisotropies

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Abstract

The mixed-spin ferrimagnetic Ising system consists of two-dimensional sublattices *A* and *B* with spin values $s_A = -1$ and $s_B = 5/2$ respectively .By used the mean-field approximation MFA of Ising model to find magnetism(m_B, m_A).In order to determined the best stabile magnetism , Gibbs free energy employ a variational method based on the Bogoliubov inequality .The ground-state (Phase diagram) structure of our system can easily be determined at $T = 0$, we find six phases with different spins values depend on the effect of a single-ion anisotropies D_B, D_A .these lead to determined the second , first orders transition ,and the tricritical points as well as the compensation phenomenon .

Key words: mixed-spin Ising model; ferrimagnet; single-ion anisotropy; compensation point.

Introduction:

There are many studies of mixing spin Ising systems investigated in the past for both theoretically and experimentally, since magnetic materials represented important for technological applications. The mean-field approximation (MFA)describes cooperative phenomena in which the effect of the ordering interaction represented by that of a mean field proportional to the average net magnetic moment of a magnetic system [1] . There is an interesting possibility of the existence of a compensation temperature $(T_k < T_c)$, at which the resultant magnetization vanishes [2].A. Dakhama et al [3] obtained an exact solution for the mixed spin-1/2 and spin-5/2 system showing that the presence of second-neighbor interaction is essential for the occurrence of a compensation point . Monte-Carlo simulation results [4] of a mixed spin-2 and spin-5/2 Ising model on a layered honeycomb lattice agree with ref.[3] . The outline of this work includes, in section 2 formulation of the model and its mean-field solution . A Landau expression of the free energy in the order parameter is demanded in this section . Finally , we have discussed in subject of the phase diagrams for various values of the anisotropies , and this is the substance our paper .

Formulation of the model and its approximate solution:

The mixed-spin ferrimagnetic Ising system , we are interested in, consists of two-dimensional sublattices A and B with spin values $s_A = 1$ and $s_B = 5/2$ respectively. The system is described by the following Hamiltonian :

$$H = -J_{ij}\sum_{i,j} s_i^A s_j^B - D_A \sum_i (s_i^A)^2 - D_B \sum_j (s_j^B)^2 \quad ...(1)$$

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Where the sites of sublattice A are occupied by spin s_i^{A} taking the values of $0, \pm 1$, and the sites of sublattice B occupied by spins s_j^{B} taking the values of $\pm 1/2, \pm 3/2, \pm 5/2$. D_A, D_B are the anisotropies acting on the spin-1 and spin-5/2 respectively. J_{ij} is the exchange interaction between spins at sites I and j .

In order to derive the best possible approximation to the model for a given microscopic Hamiltonian , we employ a variational method based on the Bogoliubov inequality for Gibbs free energy [5] :

$$F \leq \Phi = F_0 + \langle H - H_0 \rangle_0 ...(2)$$

Where F is the free energy of H given by relation (1) , F_0 is the free energy of a trial Hamiltonian H_0 depending on variational parameters and $\langle ... \rangle_0$ denotes a thermal average over the ensemble defined by H_0. In this work we consider one of the simplest possible choices of H_0, namely :

$$H_0 = -\sum_i [\lambda_A s_i^A + D_A (s_i^A)^2] - \sum_j [\lambda_B s_j^B + D_B (s_j^B)^2] ...(3)$$

Where λ_A and λ_B are the two variational parameters related to the two different spins respectively .

Now , let us obtain the approximated free energy of the system considered by minimizing the right side of equation(2) with respect to variational parameters . Thus , we can evaluate the expression in Eq.(2) that one has :

$$f \equiv \frac{\Phi}{N} = -\frac{1}{2\beta}\{\ln[1 + 2e^{\beta D_A}\cosh(\frac{1}{2}\beta\lambda_A)] + \ln[2e^{25/4\beta D_B}\cosh(\frac{5}{2}\beta\lambda_B) + 2e^{9/4\beta D_B}\cosh(\frac{3}{2}\beta\lambda_B) + 2e^{1/4\beta D_B}\cosh(\frac{1}{2}\beta\lambda_B)]\} + 1/2\lambda_B m_B ...(4)$$

Where $\beta = \dfrac{1}{K_B T}$, N is the total number of sites of lattice and Z its nearest-neighbor coordination number . The sublattice magnetizations per site m_A, m_B are defined by :

$$m_A \equiv \langle s_i^A \rangle_o = \frac{2\sinh(\beta\lambda_A)}{2\cosh(\beta\lambda_A) + e^{-\beta D_A}} ...(5)$$

,

$$m_B \equiv \langle s_j^B \rangle_o = \frac{1}{2}\frac{5\sinh(\frac{5}{2}\beta\lambda_B) + 3e^{-4\beta D_B}\sinh(\frac{3}{2}\beta\lambda_B) + e^{-6\beta D_B}\sinh(\frac{1}{2}\beta\lambda_B)}{\cosh(\frac{5}{2}\beta\lambda_B) + e^{-4\beta D_B}\cosh(\frac{3}{2}\beta\lambda_B) + e^{-6\beta D_B}\cosh(\frac{1}{2}\beta\lambda_B)} ...(6)$$

Minimizing the expression (4) with respect to λ_A and λ_B , we obtain :

$$\lambda_A = ZJm_B \qquad , \lambda_B = ZJm_A ...(7)$$

Since the present model has been able to provide an insight into the nature of first and second-order phase transitions , the stable phase will be the one which minimize the free energy . Thus , the detailed analysis of the phase diagram can be determined analytically . So , we need to expand eqs.(4)-(6) close to the second-order phase transition , for example , from an ordered state to the paramagnetic one , the magnetizations m_A and m_B are very small [1] , then one has :

$$f = f_o + am_A^2 + bm_A^4 + cm_A^6 + dm_A^8 ...(8)$$

Where the coefficients f_o, a and b are given by :

$$f_o = -\frac{1}{2\beta}\ln[(1 + x_a)(x_b + y_b + z_b)] ...(9)$$

$$a = -\frac{1}{2\beta}[t^2 b_1 + \frac{1}{4}t^4 a_1 b_1^2] + \frac{1}{2}tZJb_1 ...(10)$$

With

$$t = 0.5ZJ\beta, \qquad x_a = 2e^{\beta D_A},$$
$$, x_b = 2e^{25/4\beta D_B}, \qquad y_b = 2e^{9/4\beta D_B},$$
$$z_b = 2e^{1/4\beta D_B}, \qquad a_1 = \frac{4x_a}{1+x_a}, \qquad \ldots(11)$$
$$b_1 = \frac{25x_b + 9y_b + z_b}{x_b + y_b + z_b},$$
$$b_2 = \frac{1}{2}\frac{625x_b + 81y_b + z_b}{x_b + y_b + z_b}$$

The second and first-order phase transition lines are then determined when *a*=0,*b*>0 and *a*=*b*=0 ,*c*>0 respectively [1] . Hence the points at which *a*=0 , *b*>0 and *a*=*b*=0 , *c*>0 are the critical and tricritical ones respectively .

Results and discussions:

First, let us consider the ground-state structure of our system can easily be determined from Hamiltonian (1) by comparing the energies of the corresponding configurations as shown in Fig. (1) . At zero temperature , we find six phases with different values of $\{m_A, m_B, k_A, k_B\}$, namely , the ordered Ferrimagnetic phases $O_1 \equiv \{-1, \frac{5}{2}, 1, \frac{25}{4}\}, O_2 \equiv \{-1, \frac{3}{2}, 1, \frac{9}{4}\}, O_3 \equiv \{-1, \frac{1}{2}, 1, \frac{1}{4}\}$ and disordered phases $D_1 \equiv \{0,0,0,\frac{25}{4}\}, D_2 \equiv \{0,0,0,\frac{9}{4}\}, D_3 \equiv \{0,0,0,\frac{1}{4}\}$, where the parameters k_A and k_B defined by :

$$k_A = \langle (s_i^A)^2 \rangle, \qquad k_B = \langle (s_j^B)^2 \rangle ...(12)$$

the ground-state phase diagram is easily determined from Hamiltonian (1) by comparing the ground state energies of the different phases , the phase diagrams are numerically analyzed in the (D_A, T)and (D_B, T)phases by using Eq.(1).

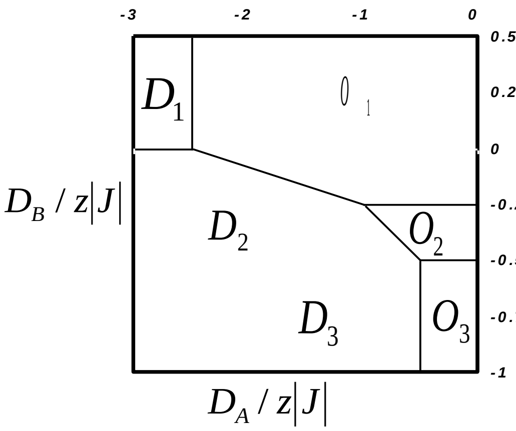

Fig.1. Ground state phase diagram of the mixed spin-1 and spin-5/2 Ising ferrimagnet system with the coordination number *Z* and different single-ion anisotropies D_A and D_B . The six phases: ordered O_1,O_2,, and O_3 and disordered D_1,D_2,, and D_3 are separated by thin lines .

In fig.(2)the phase diagrams of $K_B T_C / z|J|$ versus $D_A / z|J|$ are shown for selected values of $D_B / z|J|$. Solid and light dashed lines are used for the second and first-order transition, respectively, while the heavy dashed curve represents the positions of tricritical points. The second-order phase transition lines are easily obtained from Eq.(10) by setting $a = 0$,however , the first-order phase transitions must be determined by comparing the corresponding Gibbs free energies of the various solutions of Eq.(5) and (6) for the pair (m_A, m_B).In particular , the values of the transition temperature in the absence of anisotropies ($D_A = D_B = 0$)are $K_B T_C / z|J|$=0.6987,0.930433 and1.396067 for Z=3,4 and 6 ,respectively. These results may be compared to those of the effective-field theory with correlations [6].

The critical points at which the phase transitions change from second to first order ,are determined from Eq. (10) by setting a=0. We note that for $D_B \to +\infty$, when the

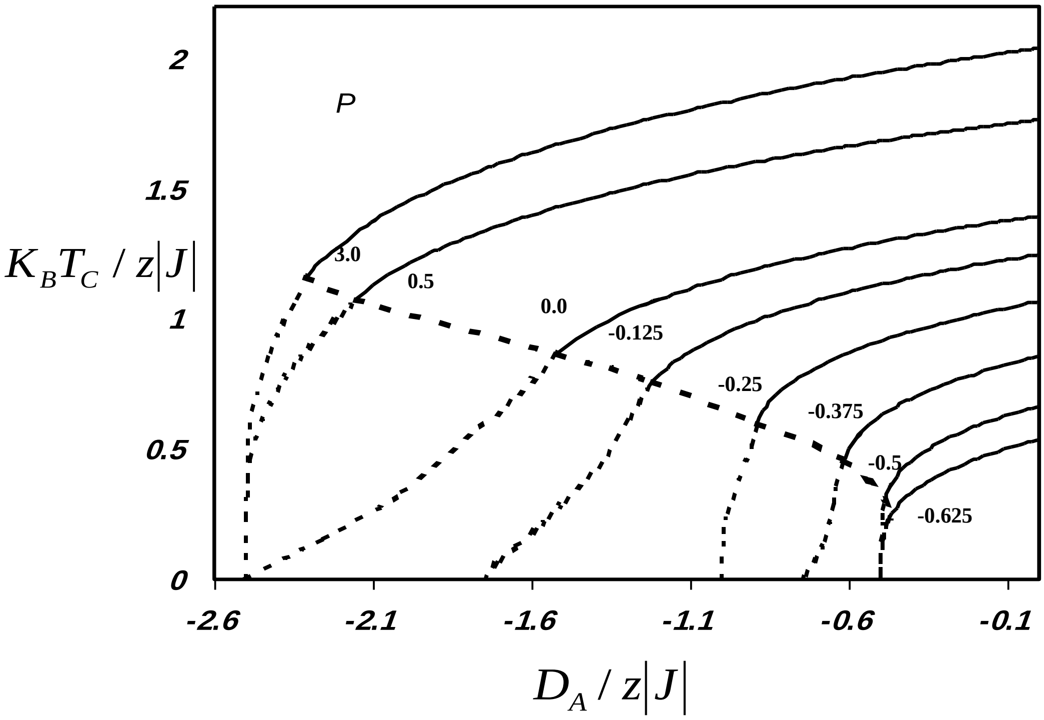

Fig. 2. Phase diagram in the (D_A,T) plane for the mixed-spin Ising ferrimagnet with the coordination number Z , when the value of D_B is changed . The solid and light dashed lines indicate second and first-order phase transitions ,While the heavy dashed line represents the position of tricritical points. ***P*** is the paramagnetic phase .

spin 5/2 behaves like a two level system with $S_j^B = \pm 5/2$, the coordinates ($D_A / z|J|, K_B T / z|J|$)of the tricritical point are (-2.30375,1.1625). On the other hand , for $D_B \to -\infty$, the $S_j^B = \pm 5/2$ states are suppressed and the system becomes equivalent to a mixed spin ½ and spin 1 Ising model [7] with the tricritical point located at (-0.45,0.2775). for its reason the coordinates of the tricritical point in the limit of large positive D_B are five times higher than those for large negative D_B .Fig. (3) shown the phase diagrams in the (D_A, T) plane for different values of D_A .For $D_A / z|J| > -0.4925$ the phase diagram are topologically to that of the spin 5/2 Blume-capel model which does not include any tricritical point[8].

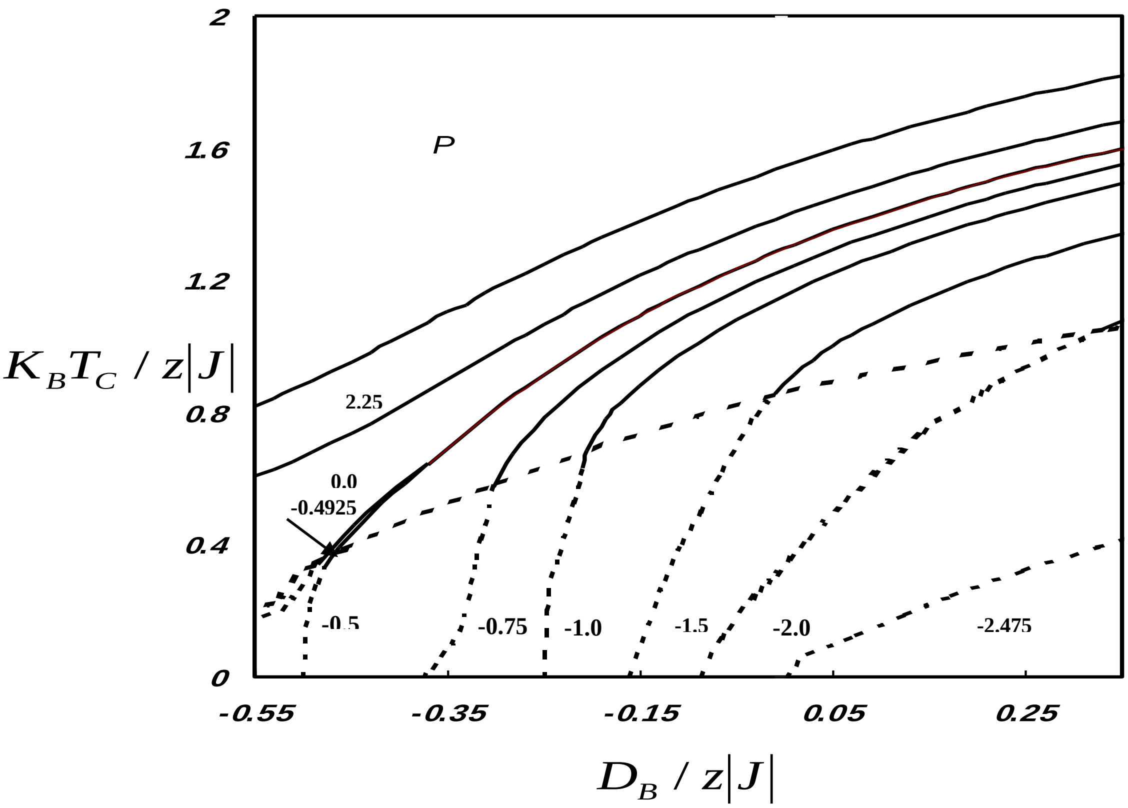

Fig. 3. Phase diagram in the (D_B,T) plane for the mixed-spin Ising ferrimagnet with the coordination number Z , when the value of D_A is changed . . The solid and light dashed lines indicate second and first-order phase transitions ,While the heavy dashed line represents the position of tricritical points. ***P*** is the paramagnetic phase .

When $D_A / z|J| \leq -0.4925$, a new type of phase diagram is achieved with a first-order transitions segment at lower temperatures and a segment of second-order transitions at higher temperatures. As $D_A / z|J|$ is lowered from –0.4925, the O_3 phase region becomes narrow and simultaneously , the tricritical point shifts towards the less negative values of $D_B / z|J|$ and the higher temperatures. At $D_A / z|J| = -0.5$, the O_3 phase disappears in agreement with the ground-state phase diagram (Fig.1) and we obtain , for $-2.30375 < D_B / z|J| \leq -0.5$,the ferrimagnetic O_1 and paramagnetic P phase that are separated by both second-and first-order transition lines. However, at $D_A / z|J| \approx -2.30375$ the second-order transition segment shrinks to zero and thus , for $-2.30375 < D_B / z|J| \leq -0.5$,the $O_1 - P$ transition is first order only.

Conclusions:

The mean-field approximation has been used in this treatment. The phase diagram of the mixed spin-1 and spin-5/2 Ising Ferrimagnetic system with different single-ion anisotropies has been determined . The magnetic properties of the system have been found by solving the general expressions numerically. Furthermore, the magnetization curves have exhibited some characteristics different from the corresponding mixed spin-1 and spin-3/2 system. On the other hand, the phase diagram at low-temperature and the sublattice magnetizations of the present work have shown a number of interesting behaviors. We hope that our present results may be helpful when the experimental data of Ferrimagnetic materials are analyzed .

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دراسة الحالة الطورية لنظام فيري مغناطيسي خليط من نوعين من المواد باستخدام نموذج أيزنك

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الخلاصة:

تم في هذا البحث دراسة نظام فيري مغناطيسي خليط من شبكتين فرعيتين B,A ذوات قيم برم $S_j^B = -5/2, S_i^A = -1$ على التوالي , حيث استخدم تقريب متوسط المجال لنموذج أيزنك لإيجاد دوال المغنطة m_B, m_A. ولإيجاد القيم المستقرة للمغنطة تم اشتقاق دالة الطاقة الحرة للنظام باستخدام لا متساوية بوكولييوف . تم وضع مخطط الحالة الأرضية (مخطط الحالة الطورية) عند $T = 0$, حيث ظهر هنالك ستة أطوار بقيم مختلف للإبرام اعتمادا على تغير قيم التباين المغناطيسي D_B, D_A. ومن خلال ذلك تم التعرف على التحولات الطورية من الدرجة الثانية والأولى والنقاط الثلاثية وكذلك نقاط الاعتدال عند $T > 0$.