

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 using the mean-field approximation MFA of Ising model to find magnetism (m_B, m_A). In order to determine the best stable 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 determine 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 of 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:

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

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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] :

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

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 $\langle \dots \rangle_0$ 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 :

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

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 :

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

Where $\beta = \frac{1}{K_B T}$, 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 :

$$m_A \equiv \langle s_i^A \rangle_0 = \frac{2 \sinh(\beta\lambda_A)}{2 \cosh(\beta\lambda_A) + e^{-\beta D_A}} \dots (5)$$

$$m_B \equiv \langle s_j^B \rangle_0 = \frac{1}{2} \frac{5 \sinh(\frac{5}{2}\beta\lambda_B) + 3e^{-4\beta D_B} \sinh(\frac{3}{2}\beta\lambda_B) + e^{-6\beta D_B} \sinh(\frac{1}{2}\beta\lambda_B)}{\cosh(\frac{5}{2}\beta\lambda_B) + e^{-4\beta D_B} \cosh(\frac{3}{2}\beta\lambda_B) + e^{-6\beta D_B} \cosh(\frac{1}{2}\beta\lambda_B)} \dots (6)$$

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

$$\lambda_A = ZJm_B, \quad \lambda_B = ZJm_A \dots (7)$$

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 :

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

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

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

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

With

$$t = 0.5 Z J \beta, \quad x_a = 2e^{\beta D_A},$$

$$, x_b = 2e^{25/4 \beta D_B}, \quad y_b = 2e^{9/4 \beta D_B},$$

$$z_b = 2e^{1/4 \beta D_B}, \quad a_1 = \frac{4x_a}{1+x_a}, \quad \dots (11)$$

$$b_1 = \frac{25x_b + 9y_b + z_b}{x_b + y_b + z_b},$$

$$b_2 = \frac{1}{2} \frac{625x_b + 81y_b + z_b}{x_b + y_b + z_b}$$

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

$$O_1 = \{-1, \frac{5}{2}, 1, \frac{25}{4}\}, O_2 = \{-1, \frac{3}{2}, 1, \frac{9}{4}\}, O_3 = \{-1, \frac{1}{2}, 1, \frac{1}{4}\}$$

and disordered phases

$$D_1 = \{0,0,0, \frac{25}{4}\}, D_2 = \{0,0,0, \frac{9}{4}\}, D_3 = \{0,0,0, \frac{1}{4}\},$$

where the parameters k_A and k_B defined by :

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

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).

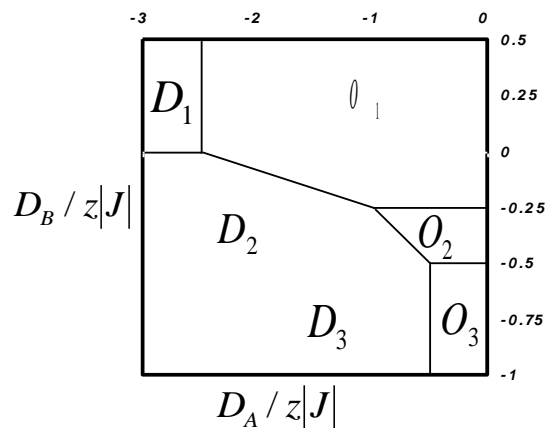


Fig.1. Ground state phase diagram of the mixed spin-1 and spin-5/2 Ising ferrimagnet system with the coordination number Z and different single-ion anisotropies D_A and D_B . The six phases: ordered $O_1, O_2,$ and O_3 and disordered $D_1, D_2,$ and D_3 are separated by thin lines.

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 $K_B T_C / z|J| = 0.6987, 0.930433$ and 1.396067 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 $D_B \rightarrow +\infty$, when the

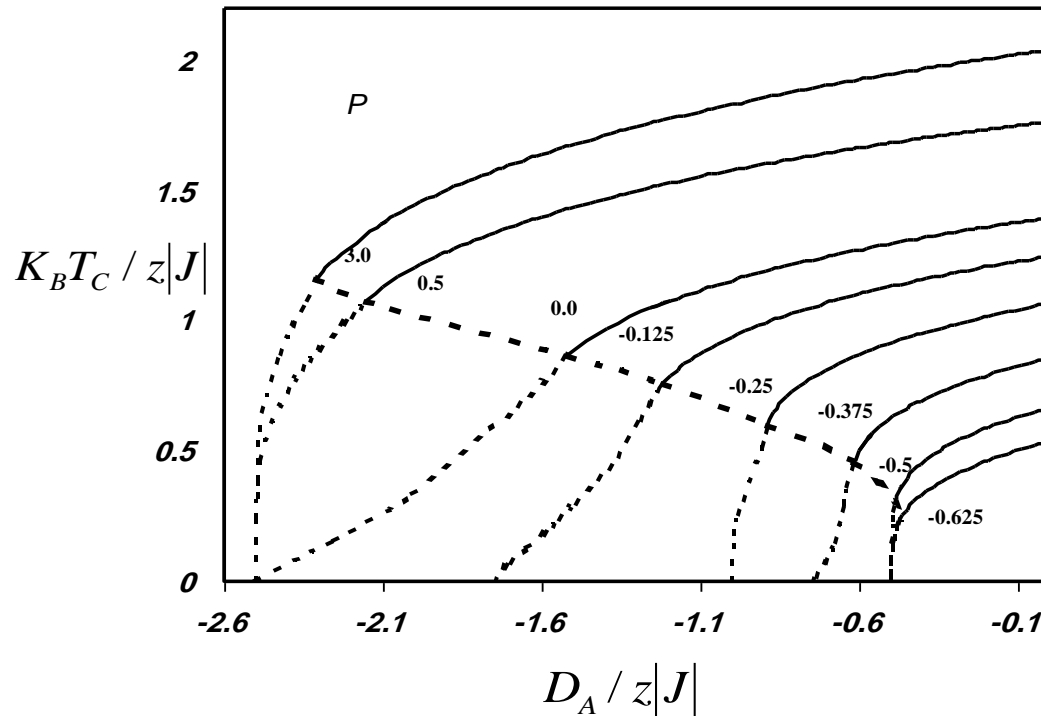


Fig. 2. Phase diagram in the (D_A, T) plane for the mixed-spin Ising ferrimagnet with the coordination number Z , when the value of D_B is changed . The solid and light dashed lines indicate second and first-order phase transitions ,While the heavy dashed line represents the position of tricritical points. 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 $D_B \rightarrow -\infty$, the $S_j^B = \pm 5/2$ states are suppressed and the system becomes equivalent to a mixed spin $1/2$ 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].

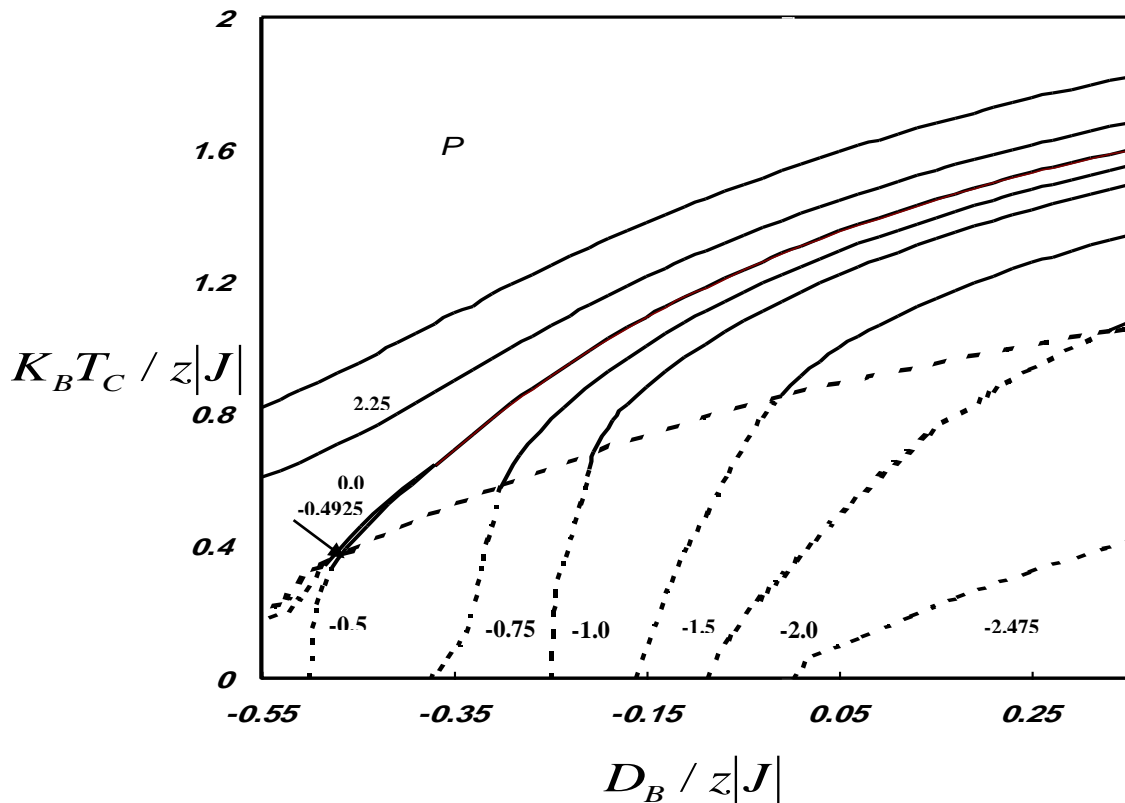


Fig. 3. Phase diagram in the (D_B, T) plane for the mixed-spin Ising ferrimagnet with the coordination number Z , when the value of D_A is changed. . The solid and light dashed lines indicate second and first-order phase transitions, While the heavy dashed line represents the position of tricritical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

References:

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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 . وإيجاد القيم المستقرة للمغنطة تم اشتقاق دالة الطاقة الحرة للنظام باستخدام لا متساوية بوكوليوف. 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 $T > 0$.