Phase Diagram of the mixed spin-2 and spin-5/2 Ising system with two different single-ion anisotropies

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Abstract

In this paper we present a study of the effects of two different single-ion anisotropies in the phase diagram and in the compensation temperature of the mixed spin-2 and spin-5/2 Ising ferrimagnetic system. We employed the mean-field theory based on the Bogoliubov inequality for the Gibbs free energy. Also we found the Landau expansion of the free energy in the order parameter to describe the phase diagrams. In the plane critical temperature versus single-ion anisotropy the phase diagram displays tricritical behavior. The critical and compensation temperatures increase when the single-ion anisotropies increase.

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I. INTRODUCTION

In the last five decades, the Ising model has been one of the most largely used to describe critical behavior of several systems in the nature. In particular, in the physics of the condensed matter it is important to describe critical behavior and other thermodynamics properties of a variety of physical systems (disordered system, spins glass, random field Ising model, etc.). Recently, several extensions have been made in the spin—1/2 Ising model to describe a wide variety of physical systems. For example, the models consisting of mixed spins of different magnitudes are interesting extensions, which are the so-called mixed-spin Ising models.

The researches in ferrimagnetic materials are of great interest due to their possible technological applications, as well as of the academic point of view. These materials are modeled by mixed-spin Ising model, which can be constituted by several combinations of spins (spin-1/2, spin-1), (spin-1/2, spin-3/2), (spin-1, spin-3/2), (spin-2, spin-3/2), (spin-2, spin-5/2). The interest in studying magnetic properties of some types of ferrimagnetism, namely the molecular-based magnetic materials [1–3], is due to its less translational symmetry than to their single-spin counterparts since they consist of two interpenetrating sublattices. The bimetallic chain complex 

II. THE MODEL AND CALCULATION

The mixed-spin ferrimagnetic Ising system consists of two interpenetrating square sublattices (A and B) with spin 

\[ S_A = \pm 1, \pm 2 \]

and spin 

\[ S_B = \pm 1/2, \pm 3/2, \pm 5/2 \].

In each site of the lattice there is a single-ion anisotropy (\( D_A \) in the sublattice A and \( D_B \) in the sublattice B) acting in the spin-2 and spin-5/2 Ising ferrimagnetic system. The outline of the remainder of the paper is as follows: In Section II, the model is introduced and we have obtained analytical expressions for free-energy, equations of state. We also have found the Landau expansion of the free energy in the order parameter. In Section III, we present the results and discussions about the phase diagrams and the compensation temperature. Finally, in Section IV we present our conclusions.

In order to derive the analytical expressions for free-energy and equations of state, we employed the variational method based on the Bogoliubov inequality for the Gibbs free energy

\[
G(\mathcal{H}) \leq G_0(\mathcal{H}_0) + \langle \mathcal{H} - \mathcal{H}_0(\eta) \rangle_0 = \Phi(\eta),
\]
calculations, we choose the simplest trial Hamiltonian, which is given by

\[ \mathcal{H}_0 = -\sum_{i \in A} [D_A(S_i^A)^2 + \eta_A S_i^A] - \sum_{j \in B} [D_B(S_j^B)^2 + \eta_B S_j^B], \]  

(3)

where \( \eta_A \) and \( \eta_B \) are variational parameters related to the two different spins. Through this approach, we found the free energy and the equations of state (sublattice magnetization per site \( m_A \) and \( m_B \)):

\[
g = \frac{\phi}{N} = -\frac{1}{2\beta} \ln \left[ 2 \exp \left( 4\beta D_A \right) \cosh \left( 2\beta \eta_A \right) + 2 \exp \left( \beta D_A \right) \cosh \left( \beta \eta_A \right) + 1 \right] 
- \frac{1}{2\beta} \ln \left[ 2 \exp \left( \frac{25}{4} \beta D_B \right) \cosh \left( \frac{5}{2} \beta \eta_B \right) + 2 \exp \left( \frac{9}{4} \beta D_B \right) \cosh \left( \frac{3}{2} \beta \eta_B \right) 
+ 2 \exp \left( \frac{1}{4} \beta D_B \right) \cosh \left( \frac{1}{2} \beta \eta_B \right) \right] 
- \frac{1}{2} J z m_A m_B + \frac{1}{2} \eta_A m_A + \frac{1}{2} \eta_B m_B,
\]  

(4)

where \( g = \frac{\phi}{N}, \beta = 1/k_B T, N \) is the total number of sites of the lattice and \( z \) is the coordination number. The sublattice magnetization per site \( m_A \) and \( m_B \) are defined by \( m_A = \langle S_i^A \rangle_0 \) and \( m_B = \langle S_i^B \rangle_0 \), thus

\[
m_A = \frac{2 \sinh \left( 2\beta \eta_A \right) + \exp \left( -3\beta D_A \right) \sinh \left( \beta \eta_A \right)}{\cosh \left( 2\beta \eta_A \right) + \exp \left( -3\beta D_A \right) \cosh \left( \beta \eta_A \right) + \frac{1}{2} \exp \left( -4\beta D_A \right)},
\]  

(5)

and

\[
m_B = \frac{1}{2} \left[ \exp \left( -3\beta D_B \right) \sinh \left( \frac{1}{2} \beta \eta_B \right) + 3 \exp \left( -4\beta D_B \right) \sinh \left( \frac{3}{2} \beta \eta_B \right) + 5 \sinh \left( \frac{5}{2} \beta \eta_B \right) \right]
\cdot
\exp \left( -3\beta D_B \right) \cosh \left( \frac{1}{2} \beta \eta_B \right) + \exp \left( -4\beta D_B \right) \cosh \left( \frac{3}{2} \beta \eta_B \right) + \cosh \left( \frac{5}{2} \beta \eta_B \right).
\]  

(6)

Minimizing the free energy in terms of the variational parameters \( \eta_A \) and \( \eta_B \), we have obtained

\[
\eta_A = J z m_B, \quad \eta_B = J z m_A.
\]  

(7)

Therefore, we can get the generic mean-field equations (4-7), which provide the magnetic properties of ferrimagnetic system. Since these equations (5-7) have in general several solutions for the pair \( (m_A, m_B) \), the stable phase will be one which minimizes the free energy. The detailed phase diagram is determined by numerical analysis, but some features of the phases diagram can be obtained analytically. Therefore, close to the second-order phase transition from an ordered state \( (m_A \neq 0 \text{ and } m_B \neq 0) \) to a disordered state \( (m_A = 0 \text{ and } m_B = 0) \). The magnetization \( m_A \) and \( m_B \) are very small, so we can expand the equations (11-12) to obtain a Landau-like expansion:

\[
g = A_0 + A_2 m_A^2 + A_4 m_A^4 + A_6 m_A^6 + \cdots,
\]  

(8)

where the expansion coefficients are given by

\[
A_0 = -\frac{1}{2\beta} \ln [(1 + y_a + x_a)(z_b + y_b + x_b)],
\]  

(9)

\[
A_2 = \frac{1}{2\beta} \left[ \frac{t^2}{4} a_1 - \frac{t^2}{8} a_2 - \frac{t^4}{32} a_1^2 b_1 \right],
\]  

(10)

\[
A_4 = \frac{1}{2\beta} \left[ \frac{t^4}{768} c_1^2 c_1 + \frac{t^3}{192} c_2 a_1 a_2 + \frac{t^2}{96} c_3 \right],
\]  

(11)

\[
A_6 = \frac{1}{2\beta} \left[ \frac{t^4}{11520} (c_4 + 6 t^6 c_5) + t^5 \left( \frac{2 a_2}{18423} c_2 (3a_1 - a_3) - \frac{c_5}{7680} a_2 a_1 \right) + \frac{t^6 c_2}{18432} \left( a_4 - 3a_1 a_2^2 \right) + \frac{t^8}{245760} c_6 \right],
\]  

(12)

with \( t = \beta J z \), and

\[
x_a = 2 e^{4\beta D_A} ; \quad y_a = 2 e^{3\beta D_A} ; \quad z_{a2} = e^{-6\beta D_B} ; \quad z_{a1} = e^{-4\beta D_B} ;
\]

\[
x_b = 2 e^{6\beta D_B} ; \quad y_b = 2 e^{4\beta D_B} ; \quad z_{b2} = 2 e^{2\beta D_B} ; \quad t = z J \beta,
\]  

(13)
\[ a_1 = \frac{z_{b_2} + 9z_{b_1} + 25}{z_{b_2} + z_{b_1} + 1}, \quad a_2 = \frac{4x_a + y_a}{x_a + y_a + 1}, \quad b_1 = \frac{25x_b + 9y_b + z_b}{x_b + y_b + z_b}, \]
\[ a_3 = \frac{z_{b_2} + 81z_{b_1} + 625}{z_{b_2} + z_{b_1} + 1}, \quad a_4 = \frac{16x_a + y_a}{x_a + y_a + 1}, \quad b_2 = \frac{625x_b + 81y_b + z_b}{x_b + y_b + z_b}, \]
\[ a_5 = \frac{z_{b_2} + 729z_{b_1} + 15625}{z_{b_2} + z_{b_1} + 1}, \quad a_6 = \frac{64x_a + y_a}{x_a + y_a + 1}, \quad b_3 = \frac{15625x_b + 729y_b + z_b}{x_b + y_b + z_b}, \]
\[ c_1 = \frac{t^4}{8}a_1^3(a_2^2 - a_4), \quad c_2 = \frac{t^3}{2}(3a_1^2 - a_3), \quad c_3 = \frac{t^2}{4}(3b_1^2 + 4a_3 - 12a_1^2 - b_2), \]
\[ c_4 = \frac{t^2}{4}(-b_1 + 15b_1b_2 - 30 - b_1), \quad c_5 = \frac{t^3}{4}(-15a_3a_1 + a_5 + 30a_1^3), \]
\[ c_6 = \frac{t^4}{12}(-a_6a_1^6 - 30(a_2a_1^2)^3 + 15a_2a_4a_1^6). \]

III. RESULTS AND DISCUSSIONS

The phase diagrams were constructed according to the following routine: i) numerical solutions of \( A_2 = 0 \) and \( A_4 > 0 \) provide second-order transition lines. ii) \( A_2 = 0, A_4 = 0 \) and \( A_6 > 0 \) determines the tricritical points. iii) The first-order transition lines are determined by comparing the corresponding Gibbs free energies of the various solutions of equations (5) and (6) for the pair \((m_A, m_B)\). Even so, we have also analysed that \( A_6 > 0 \) in all \( T, D_A, D_B \) space.

The particular case \( D_A = D_B = 0 \), the critical temperature is determined by taking \( m_A \to 0 \) and \( m_B \to 0 \), or \( A_2 = 0 \) and \( D_A = D_B = 0 \), thus \( k_B T_c/J = 9.6609 \).

A. The ground-state

The ground-state phase diagram (see Fig. 1) is determined from the Hamiltonian (1) by comparing the ground-state energies of the different phases. At zero temperature, the structure of the ground state of the system consists of six phases with different values of \( \{m_A, m_B, q_A, q_B\} \), namely the ordered ferrimagnetic phases

\[ O_1 = \{-2, \frac{5}{2}, 4, \frac{25}{4}\}, \quad O_2 = \{-1, \frac{5}{2}, 1, \frac{25}{4}\}, \]
\[ O_3 = \{-2, \frac{3}{2}, 4, \frac{9}{4}\}, \quad O_4 = \{-1, \frac{3}{2}, 1, \frac{9}{4}\}, \]
\[ O_5 = \{-2, \frac{1}{2}, 4, \frac{1}{4}\}, \quad O_6 = \{-1, \frac{1}{2}, 1, \frac{1}{4}\}, \]

where \( q_A = \langle (S_i^A)^2 \rangle \) and \( q_B = \langle (S_i^B)^2 \rangle \). The energies are given by

\[ E_1 = -\left(\frac{5}{2}Jz + 2D_A + \frac{25}{8}D_B\right), \quad E_2 = -\left(\frac{5}{4}Jz + \frac{1}{2}D_A + \frac{25}{8}D_B\right), \]
\[ E_3 = -\left(\frac{3}{2}Jz + 2D_A + \frac{9}{8}D_B\right), \quad E_4 = -\left(\frac{3}{4}Jz + \frac{1}{2}D_A + \frac{9}{8}D_B\right), \]
\[ E_5 = -\left(\frac{1}{2}Jz + 2D_A + \frac{1}{8}D_B\right), \quad E_6 = -\left(\frac{1}{4}Jz + \frac{1}{2}D_A + \frac{1}{8}D_B\right). \]
that the coordinates of the tricritical point in the limit of large positive temperatures, for all positive and negative values of $kT_\perp$, the system presents tricritical behavior. Additionally, the diagram shows that when $D_B/|J| \to +\infty$, the mixed spin Ising system behaves like a two-level system since the spin-$5/2$ behaves like $S^B = \pm 5/2$. Nevertheless, in case that $D_B/|J| \to -\infty$, the $S^B = \pm 5/2$ states are suppressed and the system becomes equivalent to a mixed spin-$1/2$ and spin-$2$ Ising model. So, this is the reason that the coordinates of the tricritical point in the limit of large positive $D_B/|J|$ are well higher than those for large negative $D_B/|J|$. For the special case with equal anisotropic fields ($D_A/|J| = D_B/|J| = 0$), the critical temperature is $k_B T_c/|J| = 9.6609$, and the location of the tricritical point is $k_B T_c/|J| = 3.3833$, $D_A/|J| = -6.2150$, for $z = 4$.

In Fig. 3, it is shown the phase diagram of $k_B T_c/|J|$ versus $D_B/|J|$ for various values of $D_A/|J|$. In the case of $D_A/|J| > -1.8842$ the phase transitions are only of second-order (solid lines) for any values of $D_B/|J|$. The value of the critical temperature increases when $D_B/|J|$ and $D_A/|J|$ also increase. Still, in range $-1.8842 < D_A/|J| < -9.0$, the phase transitions are of second-order in the high temperatures region (solid lines) and of first-order (light dashed lines) in the low temperatures region. One heavy dotted curve of tricritical points separates the second from the first-order transition lines.

One interesting feature shown in the diagram of the Fig. 3, refers to the fact that the phase transitions are only of first-order when the values of $D_A/|J| < -9.0$. All lines that start below the heavy dotted line will necessarily be only of first-order phase transition. Again, in this space ($D_B/|J|$, $k_B T/|J|$), the system presents tricritical behavior.

These results may be compared to those obtained in the paper [13], which it has an error in equation (4) and consequently in the equation (8). These errors led to very different phase diagrams at temperatures above zero.
Figure 2: Phase diagram in the \( (D_A/|J|, k_B T/|J|) \) plane for the mixed-spin Ising ferrimagnet with the coordination number \( z = 4 \), for several values of \( D_B/|J| \). The solid and light dashed lines, respectively, indicate second- and first-order phase transitions, while the heavy dashed line represents the positions of tricritical points.

Figure 3: Phase diagram in the \( (D_B/|J|, k_B T/|J|) \) plane for the mixed-spin Ising ferrimagnet with the coordination number \( z = 4 \), for several values of \( D_A/|J| \). The solid and light dashed lines, respectively, indicate second- and first-order phase transitions, while the heavy dashed line represents the positions of tricritical points.

C. Compensation temperature

The present mixed-spin system can exhibit compensation points, and to show this fact, we will consider \( J < 0 \). The signs of the sublattice magnetizations are different since we are taking into account that in the ferrimagnetic case the system consists of two interpenetrating square sublattices (A and B) with spin-2 and spin-5/2. Thus, it is possible that there are a compensation temperature \( T_{\text{comp}} \) with \( T_{\text{comp}} < T_c \). So, the total magnetization per site \( M = (m_A + m_B)/2 \) is equal to zero, same that \( m_A \neq 0 \) and \( m_B \neq 0 \).

In Fig. 4, we present the diagram \( T_c \) and \( T_{\text{comp}} \) versus \( D_A/|J| \), and for some selected values of \( D_B/|J| \). The diagram shows that there are compensation points in the range \( 2.5339 < D_B/|J| < -10.0 \) and for \( D_A/|J| > -2.50 \), which are indicated by dotted lines, while solid lines indicate critical temperature. The inset in Fig. 4 exhibits some
Figure 4: The critical $T_c$ and compensation $T_{comp}$ temperatures as a function of the single-ion anisotropy $D_A/|J|$, and for several values of $D_B/|J|$. The solid and dotted curves represent the critical temperature and compensation temperature, respectively. The inset shows a magnification of the region closed where the compensation and critical temperatures are together for $D_B/|J| = -10.0$. Temperatures are measured in units of $|J|/k_B$.

compensation points in case of $D_B/|J| = -10.0$. The Fig. 5 exhibits the diagram $T_c$ and $T_{comp}$ versus $D_B/|J|$, for the some selected values of $D_A/|J|$. This figure only confirms the information shown in Fig. 4, ie, there is compensation temperature in the range $2.5339 < D_B/|J| < -10.0$ and $D_A/|J| > -2.5$.

Figure 5: The critical $T_c$ and compensation $T_{comp}$ temperatures as a function of the single-ion anisotropy $D_B/|J|$, and for several values of $D_A/|J|$. The solid and dotted curves represent the critical temperature and compensation temperature, respectively. Temperatures are measured in units of $|J|/k_B$.

IV. CONCLUSIONS

In this paper, we have studied the effects of two different anisotropies in the phase diagram and in the compensation temperature of the mixed spin-2 and spin-5/2 ferrimagnetic Ising system by using the mean field theory based on the Bogoliubov inequality. The phase diagrams are shown in the critical temperature versus single ions anisotropies plane. The system presents tricritical behavior, ie, the second-order phase transition line is separated of the first-order transition line by a tricritical point. Additionally, we also observed compensation temperatures. So, in conclusion, we can say that such a system may exhibit tricritical behavior and compensation temperatures due to the two different anisotropies.
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[1] O. Kahn, Molecular Magnetism, VCH, New York, (1993).
[2] T. Kaneyoshi and Y. Nakamura, J. Phys.: Condens. Matter 10, 3003 (1998).
[3] T. Kaneyoshi and Y. Nakamura, S. Shin, J. Phys.: Condens. Matter 10, 7025 (1998).
[4] M. Drillon, E. Coronado, D. Beltran, and R. Georges, J. Chem. Phys. 79, 449 (1983)
[5] A. Bobáč, Physica A 258, 140 (1998).
[6] H. F. Verona de Resende, F. C. Sá Berreto, and J. A. Plascak, Physica A 149A, 606 (1988).
[7] E. Albayrak and M. Keskini, J. Magn. Magn. Mater. 261, 196 (2000).
[8] T. Kaneyoshi, J. Phys. Soc. Japan 56, 2675 (1987).
[9] T. Kaneyoshi, Physica A 153, 556 (1988).
[10] T. Kaneyoshi, J. Magn. Magn. Mat. 92, 59 (1990).
[11] A. Benyoussef, A. El Kenz, and T. Kaneyoshi, J. Magn. Magn. Mat. 131, 173 (1994).
[12] A. Benyoussef, A. El Kenz, and T. Kaneyoshi, J. Magn. Magn. Mat. 131, 179 (1994).
[13] H. K. Mohamad, E. P. Domashevskaya, and A. F. Klinskikh, Physica A 388, 4713 (2009).
[14] A. Bobák and M. Jurčišin, Physica A 240, 647 (1997).
[15] D. C. de Oliveira, A. A. P. da Silva, D. F. de Albuquerque, and A. S. de Arruda, Physica A 386, 205-211 (2007).
[16] D. F. de Albuquerque, S. R. L. Alves, and A. S. de Arruda, Physics Letters A 346, 128-132 (2005).
[17] T. Kaneyoshi and J. C. Chen, J. Magn. Magn. Mater. 98, 201 (1991).
[18] W. G. Zhu and M. H. Ling, Commun. Theor. Phys. 51, 756 (2009).
[19] S. G. A. Quadros and S. R. Salinas, Physica A 206, 479 (1994).
[20] G. M. Zhang and C. Z. Yang, Phys. Rev. B 48, 9452 (1993).
[21] G. M. Buendia and M. A. Novotny, J. Phys.: Condens. Matter 9, 5951 (1997).
[22] G. M. Buendia and J. A. Liendo, J. Phys.: Condens. Matter 9, 5439 (1997).
[23] M. Godoy and W. Figueiredo, Phys. Rev. E 61, 218 (2000); 65, 026111 (2002); 66, 036131 (2002).
[24] G. Wei, Q. Zhang, and Y. Gu, J. Magn. Magn. Mater. 301, 245 (2006).
[25] G. Wei, Y. Gu, and Jing Liu, Phys. Rev. B 74, 024422 (2006).
[26] M. Žukovič, A. Bobáč, Physica A 389, 5401 (2010).
[27] M. Žukovič and A. Bobáč, J. Magn. Magn. Mater. 322, 2868 (2010).
[28] R. A. Yessoufou, S. Bekhechi, and F. Hontinfinde, Eur. Phys. J. B 81, 137 (2011).
[29] L. L. Goncalves, Phys. Scr. 32, 248 (1985).
[30] L. L. Goncalves, Phys. Scr. 33, 192 (1986).
[31] O. F. Abubrig, D. Horvath, A. Bobáč, and M. Jascur, Physica A 296, 437 (2001).