The Effect of the Crystal Field Interaction on the Critical Temperatures and the Sublattice Magnetizations of a Mixed Spin-3/2 and Spin-5/2 Ferrimagnetic System

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Abstract—The influence of the crystal field interactions on the mixed spin-3/2 and spin-5/2 ferrimagnetic Ising system is considered by using the mean field theory based on Bogoliubov inequality for the Gibbs free energy. The ground-state phase diagram is constructed, the phase diagrams of the second-order critical temperatures are obtained, and the thermal variation of the sublattice magnetizations is investigated in detail. We find some interesting phenomena for the sublattice magnetizations at particular values of the crystal field interactions.

Keywords—Crystal field, Ising system, Ferrimagnetic, magnetization, phase diagrams.

I. INTRODUCTION

The Ising model, with high and mixed spins, is an interesting subject of study because of its observed critical behaviors. The two sublattice mixed Ising ferrimagnetic systems have been of interest in the last two decades, for not only purely theoretical purposes but also because they have been proposed as possible systems to describe ferromagnetic and ferrimagnetic materials [1]. Moreover, the increasing interest in these systems is mainly related to the technological applications of these systems in the area of thermomagnetic recording [2]. Since the mixed spin Ising systems have less translational symmetry than their single spin counterparts, they exhibit many new phenomena which cannot be observed in the single-spin Ising systems and the study of these systems can be relevant for understanding of bimetallic molecular systems based magnetic materials [3].

One of the earliest and simplest of these models to be studied was the mixed spin Ising system consisting of spin-1/2 and spin-S (S > 1/2) in a uniaxial crystal field. The model for different values of S (S > 1/2) has been investigated by exact (on honeycomb lattice [4]-[6], as well as on Bethe lattice [7], [8], mean field approximation [9], effective field theory with correlations [10]-[14], cluster variational technique [15] and Monte-Carlo simulation [16]-[18]. The mixed- spin Ising systems consisting of higher spins are not without interest. Indeed, the magnetic properties of mixed spin-1 and spin-3/2 Ising ferromagnetic system with different single-ion anisotropies have been investigated with the use of an effective field theory [18], [19], mean field theory [20], a cluster variational method [21] and Monte Carlo simulation [22].

Recently, the investigations have been extended to high order mixed spin ferrimagnetic systems (mixed spin-3/2 and spin-2 ferrimagnetic system and mixed spin-3/2 and spin-5/2) in order to construct their phase diagrams in the temperature-anisotropy plane and to consider magnetic properties of these systems. Bobak and Delay investigated the effect of single-ion anisotropy on the phase diagram of the mixed spin-3/2 and spin-2 Ising system by the use of a mean-field theory based on the Bogoliubov inequality for the free energy [23]. Albyrak [24] studied the critical behaviour of the mixed spin-2 and spin-5/2 Ising ferrimagnetic system on Bethe lattice by using the exact recursion equations. Bayram Deviren et al. have used the effective field theory to study the magnetic properties of the ferrimagnetic mixed spin-3/2 and spin-2 Ising model with crystal field in a longitudinal magnetic field on a honeycomb and a square lattice [26].

In this paper, our aim is to consider a mixed spin-3/2 and spin-5/2 ferrimagnetic system within the framework of the mean-field theory based on Bogoliubov inequality for the Gibbs free energy, in order to investigate the influence of the crystal-field interaction on the critical temperatures and to find the change in the sublattice magnetizations of the system as a function of the temperature at a different values of the crystal-field interaction.

This paper is organized as follows: Section II briefly presents the mixed spin Ising model and its mean-field solution. Section III gives the results and the discussions. In Section IV the conclusion is summarized.

II. THE MODEL AND CALCULATION

We consider a mixed Ising spin-2 and spin-5/2 system consisting of two sublattices A and B, which are arranged alternately. The sublattice A are occupied by spins $S_A$ , which
take the spin values of $\pm 3/2, \pm 1/2$, while the sublattice $B$ are occupied by spins $S_j$, which take the spin values of $\pm 5/2, \pm 3/2, \pm 1/2$. In each site of the lattice, there is a single-ion anisotropy $D_A$ in the sublattices $A$ and $D_B$ in the sublattice $B$) acting in the spin-3/2 and spin-5/2. The Hamiltonian of the system according to the mean-field theory is given by

$$H = -J \sum_{i<j} (S_{iA}^x S_{jB}^y - D_A (S_{iA}^y)^2 - D_B (S_{jB}^y)^2), \quad (1)$$

where the first summation is carried out only over nearest-neighbor pairs of spins on different sublattices and $J$ is the nearest-neighbour exchange interaction.

The most direct way of deriving the mean-field theory is to use the variation principle for the Gibbs free energy,

$$G(H) \leq \Phi = G_0(H) + \langle H - H_0 \rangle, \quad (2)$$

where $\Phi$ is the true free energy of the model described by Hamiltonian given in (1), $G_0(H)$ is the model described by the trial Hamiltonian $H_0$ which depends on variational parameters and $\langle \cdot \cdot \cdot \rangle_0$ denotes a thermal average over the ensemble defined by $H_0$.

Now, depending on the choice of the trial Hamiltonian, one can construct approximate methods of different accuracy. However, owing to the complexity of the problem, we consider in this work the simple choice of $H_0$, namely

$$H_0 = -\sum_{i \in A} \gamma_A S_i^A + D_A (S_i^A)^2 - \sum_{i \in B} \gamma_B S_i^B + D_B (S_i^B)^2, \quad (3)$$

where $\gamma_A$ and $\gamma_B$ are the two variational parameters related to the molecular fields acting on the two different sublattices, respectively.

By evaluating (2), it is easy to obtain the expression of the free energy per site in MFA,

$$g = \frac{\Phi}{N} = \frac{-1}{2} \ln \left[ \exp \left( \frac{25}{4} \beta D_A \left[ 2 \cosh \frac{5}{2} \beta \gamma_A + \exp (-4 \beta D_A) \left( 2 \cosh \frac{3}{2} \beta \gamma_A + \exp (-6 \beta D_A) \left( 2 \cosh \frac{1}{2} \beta \gamma_A \right) \right) \right] \right] + \ln \left[ \exp \left( \frac{9}{4} \beta D_B \left[ 2 \cosh \frac{1}{2} \beta \gamma_B + \exp (-2 \beta D_B) \left( 2 \cosh \frac{1}{2} \beta \gamma_B \right) \right] \right] + \frac{1}{2} \left( zJ m_A m_B \right) \quad (4)$$

$$m_A = \frac{1}{2} \left[ \frac{5 \sinh \frac{5}{2} \beta \gamma_A + 3 \exp (-4 \beta D_A) \sinh \frac{3}{2} \beta \gamma_A + \exp (-6 \beta D_A) \sinh \frac{1}{2} \beta \gamma_A }{ \cosh \frac{5}{2} \beta \gamma_A + \exp (-4 \beta D_A) \cosh \frac{3}{2} \beta \gamma_A + \exp (-6 \beta D_A) \cosh \frac{1}{2} \beta \gamma_A } \right] \quad (5)$$

$$m_B = \frac{3 \sinh \frac{3}{2} \beta \gamma_B + \exp (-2 \beta D_B) \sinh \frac{1}{2} \beta \gamma_B }{ 2 \cosh \frac{3}{2} \beta \gamma_B + 2 \exp (-2 \beta D_B) \cosh \frac{1}{2} \beta \gamma_B } \quad (6)$$

where $\beta = 1/k_B T$, $N$ is the total number of sites of the lattice and $Z$ is the number of the nearest neighbors of every ion in the lattice $m_A$ and $m_B$ are the sublattice magnetizations per site which are defined by (5).

Now, by minimizing the free energy (4) with respect to $\gamma_A$ and $\gamma_B$, we obtain

$$\gamma_A = zJ m_B, \quad \gamma_B = zJ m_A. \quad (7)$$

The mean-field properties of the present model are then given by (4)-(7). Since (5)-(7) have in general several solutions for the pair $(m_A, m_B)$, the stable phase will be the one which minimizes the free energy. When the system undergoes the second-order transition from an ordered state ($m_A \neq 0, m_B \neq 0$), to the paramagnetic state ($m_A = 0, m_B = 0$), this part of the phase diagram can be determined analytically. Because the magnetizations $m_A$ and $m_B$ are very small in the neighborhood of second-order transition point, we can expand (4)-(6) to obtain a Landau-like expansion. In this way, critical and tricritical points are determined according to the following routine;

1) Second-order transition lines when $a=0$ and $b>0$;
2) Tricritical points, if they are exist, when $a=b=0$, and $c > 0.$
III. RESULTS AND DISCUSSIONS

A. Ground State Phase Diagram

Before going into the detailed calculation of the phase diagram of the model at higher temperature, let us first investigate the ground state structure of the model at zero temperature analytically. The ground-state phase diagram is easily determined from Hamiltonian Equation (1) by comparing the ground-state energies of the different phases, then the ground state configuration is the one with the lowest energy and each of these configurations for the given system parameters correspond to the stable states of the model which are indicated in Fig. 1.

At zero temperature, we find six phases with different values of \( \{m_A, m_B, q_A, q_B\} \), namely the ordered ferrimagnetic phases. These ordered phases are separated by first ordered lines and the values of \( \{m_A, m_B, q_A, q_B\} \) for these phases are given as following:

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

where the parameters \( q_A \) and \( q_B \) are defined by:

\[
q_A = \langle S_A^z \rangle^2 \quad \text{and} \quad q_B = \langle S_B^z \rangle^2
\]

It should be mentioned that, in this mixed-spin-system, the ground- state phase diagram exhibit no disordered phases and that the ground state phase diagram is very important in classifying the different phase regions of the model for the phase diagrams at higher temperatures.

B. Finite Temperature Phase Diagrams

In Figs. 2 and 3, the second-order critical temperature lines which separate the ordered phases, i.e. ferrimagnetic phases, from the paramagnetic phase of the mixed spin-3/2 and the spin-5/2 Ising ferrimagnetic system are depicted in the \( (D_A / z | J|, k_B T_c / z | J|) \) and \( (D_B / z | J|, k_B T_c / z | J|) \) planes for some selected values of \( D_A / z | J| \) for spin-5/2 and \( D_B / z | J| \) for spin-3/2, respectively.
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 \(D_A / z |J|\) is changed.

On the other hand, at this part, the second-order critical temperatures values decrease rapidly by decreasing the values of \(D_A / z |J|\). When \(D_A / z |J| \leq 20\) and \(D_A / z |J| \geq -20\). The saturated values of the second-order critical temperatures are shown in this figure.

For the final illustrations, let us now turn our attention to the saturated values of the critical temperatures for high values and low values of \(D_A / z |J|\) and \(D_B / z |J|\). As shown in Fig. 4, for high positive and negative values of \(D_A / z |J|\) and \(D_B / z |J|\). When \(D_A / z |J| \rightarrow \infty\) and \(D_B / z |J| \rightarrow -\infty\), the saturated value of the critical temperatures is \(k_B T_c / z |J| = 3.75\). When \(D_A / z |J| \rightarrow \infty\) and \(D_B / z |J| \rightarrow -\infty\), the saturated value of the critical temperatures is \(k_B T_c / z |J| = 2.5\). When \(D_A / z |J| \rightarrow -\infty\) and \(D_B / z |J| \rightarrow \infty\), the saturated value of the critical points is \(k_B T_c / z |J| = 0.75\). If \(D_A / z |J| \rightarrow -\infty\) and \(D_B / z |J| \rightarrow -\infty\), the saturated value is \(k_B T_c / z |J| = 0.25\).

C. Sublattice Magnetizations \(m_A\) and \(m_B\).

In this subsection, let us at first examine the temperature dependence of the sublattice magnetizations \(m_A\) and \(m_B\) for the system. The results are depicted in Figs. 5-7.

Fig. 5 shows typical sublattice magnetization curves with \(D_A / z |J| = 1.0\), and selected values of \(D_B / z |J|\). In this case, all the sublattice magnetization curves have standard characteristic convex shape. Moreover, in the present system and for all the values of the crystal field interactions \(D_A / z |J|\) and \(D_B / z |J|\), the present system exhibits second-order phase transitions only, consequently, the sublattice magnetizations decrease by increasing temperature from their
saturation values at $T = 0 \, K$ and vanish continuously at the critical temperatures $T_c$.

By comparing the values of the sublattice magnetizations at zero temperature, for different values of $D_A / |z| |J| \text{ and } D_B / |z| |J|$ in Fig. 5 with the values of the sublattice magnetizations, corresponding to the different phases and to the boundary between the phases, at the ground-state phase diagram (Fig. 1), we find that they are in agreement and every sublattice magnetization has the same saturated value at $T = 0 \, K$ as in the ground state phase diagram.

In Figs. 6 and 7, we turn our attention to the points which are located close to or at the boundaries between the phases in the ground-state phase diagram. In Fig. 6, when $D_B / |z| |J| = 1.0$ and $D_A / |z| |J| = 0.35$ (this point located in the ordered phase $O_1$ and close to the boundary between the ordered phase $O_1$ and the ordered phase $O_3$ in the ground state phase diagram, where $D_A / |z| |J| = 0.375$). In this case, the temperature dependences of $m_A$ may exhibit a rather rapid decrease (damping) from its saturation value at $T = 0 \, K$. The phenomena is further enhanced when the value of $D_A / |z| |J|$ approaches the boundary. At $D_B / |z| |J| = 0.375$ (at the boundary) and $T = 0 \, K$, the saturation value of $m_A$ is $m_A = 2.0$, which indicates that in the ground state the spin configuration of $S_j^B$ in the system consists of the mixed state; in this state half of the spins on sublattice $B$ are equal to $+5/2$ (or $-5/2$) and the other half are equal to $+3/2$ (or $-3/2$).

By further decreasing $D_A / |z| |J|$, the ground state becomes $O_3$, with $m_A = 3/2$ at $T = 0 \, K$. In this region, when $D_A / |z| |J| = 0.4$ (slightly below the boundary between the ordered phases $O_1$ and $O_3$), the thermal variation of $m_A$ exhibits an interesting feature which is the initial rise (excitation) of $m_A$ with the increase of temperature before decreasing to zero at the critical point. On the other hand, for all values of $D_A / |z| |J|$. 

![Fig. 5](image-url) Thermal variation of the sublattice magnetizations $m_A, m_B$ for the mixed-spin Ising ferrimagnet with the coordination number $z$, when the value of $D_A / |z| |J|$ is changed for fixed $D_B / |z| |J| = 1.0$.

![Fig. 6](image-url) Thermal variation of the sublattice magnetizations $m_A, m_B$ for the mixed-spin Ising ferrimagnet with the coordination number $z$, when the value of $D_B / |z| |J|$ is changed for fixed $D_A / |z| |J| = 1.0$.

In Fig. 6 and for all these values of $D_B / |z| |J|$ the sublattice magnetization $m_B$ may show normal behavior even though it is coupled to $m_A$.

When $D_B / |z| |J|$ has the values $-0.7, -0.75$ and $-0.8$ (close to and at the boundary between the ordered-phases $O_3$ and $O_5$ in the ground-state phase diagram), it is clear from Fig. 6 that the temperature dependences of $m_B$ and $m_A$ exhibit similar behaviors to the temperature dependences of $m_B$ and $m_A$ in the previous case.
When $0.1 |z| |J|$ is changed for fixed $D_z / |z| |J| = 1.0$, the sublattice magnetization $m_B$ may show normal behavior. When $D_z / |z| |J| = 1.0$, the sublattice magnetization $m_B$ may exhibit a rather rapid decrease from its saturation value ($m_B = -3/2$) at $T = 0 K$, while for the value of $D_z / |z| |J| = -1.5$ (slightly below that boundary), there is a rapid increase of $m_B$ from the saturation value ($m_B = -1/2$) with the increase in $T$.

When the value of $D_z / |z| |J| = -1.25$, the saturation value of the sublattice magnetization $m_B$ at $T = 0 K$ is ($m_B = -1.0$). It indicates that at this point, the spin configuration of $S^z$ in the ground state consists of the mixed state; half of the spins on the sublattice $B$ are equal to -3/2 (or +3/2 as well) and the other half are equal to -1/2 (or +1/2 as well). It is also seen from Fig. 7 that when $D_z / |z| |J| = -3.0$, the sublattice magnetization $m_B$ decreases normally from its saturation value ($m_B = -1/2$) to vanish at the critical temperature $T_c$. On the other hand, for all values of $D_z / |z| |J|$ the sublattice magnetization $m_A$ may show normal behavior, even though it is coupled to $m_B$.

**REFERENCES**


