The influence of the different transverse fields on the critical properties in the mixed Ising spin system with single-ion anisotropy

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Abstract. The effects of single-ion anisotropy and different sublattice transverse fields on the critical properties of the mixed Ising spin system on the square lattice are investigated within the framework of an effective field approximation. For certain values of the system parameters, tricritical points and reentrant phenomena can be observed, due to the competition between the different transverse fields and single-ion anisotropy. We present a detailed description of the phase diagram.

PACS. 75.10.Jm Quantized spin models – 75.40.Cx Static properties (order parameter, static susceptibility, heat capacities, critical exponents, etc.) – 75.50.Cc Other ferromagnetic metals and alloys

1 Introduction

In recent decades, there has been an interesting number of works dealing with critical properties of quantum spin systems. One of the simplest is the transverse Ising system, which has been introduced to explain the phase transition and the order-disorder phenomenon when the tunneling effect is present. Many authors have investigated the single spin or the mixed spin transverse Ising model under various conditions and within different approximations [1–6]. In particular, it is worth mentioning that the two sublattice mixed transverse Ising spin systems may be described by different transverse fields in the Hamiltonian. Critical properties of systems with different tunneling effects have also been studied by a variety of techniques [7–9].

On the other hand, some studies [11,14] indicate that the mixed Ising spin system with single-ion anisotropy in various conditions can show a number of interesting phenomena [10–15], such as reentrant phenomenon. A tricritical point at which the phase transition changes from second order to first order is predicted in the mixed spin-1/2 and spin-S (S = 1 or 2) with a coordination number zlarger than z = 3, when the single-ion anisotropy takes on a large negative value, although the mixed spin-1/2 and spin-3/2 system never exhibits any tricritical point [16].

The general idea is to study the critical properties of the transverse Ising system in the presence of single-ion anisotropy, and try to analyze the influences of both. In the last few years, numerous works have touched upon the single spin (S = 1) Ising ferromagnet with both transverse field and single-ion anisotropy [17, 18]. The tricritical point is predicted to disappear at a certain critical transverse field value. More recently, the present authors have analyzed the critical behaviours and magnetic properties of the mixed transverse Ising ferromagnetic (or ferri) system with single-ion anisotropy [19–21]. But these works concern only the uniform transverse field. The mixed Ising spin system with single-ion anisotropy and different transverse fields shows distinct critical properties. To our knowledge, the above subject has not yet been considered in previous literature.

The main purpose of this paper is to discuss the influence of different transverse fields on the critical properties of the mixed Ising spin-1/2 and spin-1 system with singleion anisotropy and to focus attention on the tricritical point and reentrant phenomenon. The mixed spin system has less translational symmetry than the single spin system counterpart and is well adapted to study a certain type of ferrimagnetism. The competition between two different transverse fields and single-ion anisotropy may result in some new phenomena which were not observed in the single spin Ising system [17] or in the mixed Ising spin system with the uniform transverse field [21]. The problem is studied on the basis of the effective field theory with correlations (EFT) introduced by Honmura and Kanevoshi [22]. This scheme has been successfully applied to a variety of Ising spin problems [8, 17, 19].

The structure of this paper is as follows. Section 2 is dedicated to the definition of the mixed Ising spin system with single-ion anisotropy and different transverse fields and to the exposition of the theoretical procedure.

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The detailed numerical results and discussion are presented in Section 3. Section 4 includes a conclusion of the results.

2 Theory

Let us consider the mixed Ising spin-1/2 and spin-1 system in which the different transverse fields and single-ion anisotropy are considered. This system can be described by the following Hamiltonian:

$$H = -J \sum_{i,j} \sigma_i^z S_j^z - \Omega_{1/2} \sum_i \sigma_i^x - \Omega_1 \sum_j S_j^x - D \sum_j \left(S_j^z\right)^2.$$
(1)

The underlying lattice is composed of two interpenetrating sublattices A and B. One is occupied by spin-1/2 with spin moment σ_i^z and σ_i^x at site A, while the other one is occupied by spin-1 with spin moment S_j^z and S_j^x at site B. Here J defines the interaction between the spin at site i and its neighbour located at site j. The analysis will be performed only for the simple case of nearest neighbours interaction. The quantities $\Omega_{1/2}$ and Ω_1 are the transverse field on the A and B sublattices, respectively. D is the parameter of single-ion anisotropy, assumed to be negative. The first summation runs only over all pairs of nearestneighbour sites. The second summation involves all sites of A. The third and the fourth summations involve all sites of B.

Within the EFT, we can investigate the critical properties and the averaged magnetization for the present system with a coordination number z. As was pointed out in reference [12], tricritical points occur in the mixed Ising system with single-ion anisotropy when z > 3. Here, for simplicity we will discuss the square lattice, thus z = 4. The averaged magnetizations in sublattices A and B are given by

$$\sigma = \left\langle \sigma_i^z \right\rangle = \left\langle \prod_{j=1}^4 \left\{ \left(S_j^z \right)^2 \cosh\left(J \nabla \right) + S_j^z \sinh\left(J \nabla \right) + 1 - \left(S_j^z \right)^2 \right\} \right\rangle F(x) \Big|_{x=0}, \quad (2)$$

and

$$m = \langle S_j^z \rangle$$

= $\langle \prod_{i=1}^{4} \{ \cosh\left(\frac{J}{2}\nabla\right) + 2\sigma_i^z \sinh\left(\frac{J}{2}\nabla\right) \} \rangle G(x) \big|_{x=0}$ (3)

while the quadrupolar moment is given by

$$q = \left\langle \left(S_{j}^{z}\right)^{2} \right\rangle$$
$$= \left\langle \prod_{i=1}^{4} \left\{ \cosh\left(\frac{J}{2}\nabla\right) + 2\sigma_{i}^{z} \sinh\left(\frac{J}{2}\nabla\right) \right\} \right\rangle H(x) \Big|_{x=0} \quad (4)$$

where $\nabla = \partial/\partial_x$ is a differential operator and $\langle ... \rangle$ indicates the canonical thermal average. The function F(x) is defined by

$$F(x) = \frac{1}{2} \frac{x}{\left(\Omega_{1/2}^2 + x^2\right)} \tanh\left(\frac{\beta}{2} \left(\Omega_{1/2}^2 + x^2\right)^{1/2}\right), \quad (5)$$

where $\beta = 1/k_{\rm B}T$. The functions G(x) and H(x) are defined by

$$G(x) = \sum_{n=1}^{3} \left[E(n) \left[\frac{2x}{3C} \cos \frac{(n-1)2\pi + \theta}{3} + \frac{2}{27} \frac{D^3 x - Dx^3 + (7/2)D\Omega_1^2 x}{BC} + \frac{2}{27} \frac{(n-1)2\pi + \theta}{3} \right] \right] \left[\sum_{n=1}^{3} E(n) \right]^{-1}, \quad (6)$$

and

$$H(x) = \sum_{n=1}^{3} \left[E(n) \left[\frac{2D}{9C} \cos \frac{(n-1)2\pi + \theta}{3} + \frac{2}{27} \frac{(1/2)\Omega_1^2 x^2 - D^2 x^2 + x^4 - (1/2)\Omega_1^4}{BC} + \frac{2}{37} \frac{(n-1)2\pi + \theta}{3} + \frac{2}{3} \right] \right] \left[\sum_{n=1}^{3} E(n) \right]^{-1}$$
(7)

where

$$E(n) = \exp\left[2\beta C\cos\frac{(n-1)2\pi + \theta}{3} + \frac{2\beta D}{3}\right], \qquad (8)$$

$$B = \frac{1}{9} \left[3 \left(D^2 x - x^3 \right)^2 + \frac{3}{4} D^2 \Omega_1^4 + 15 D^2 \Omega_1^2 x^2, + 9 \Omega_1^4 x^2 + 9 \Omega_1^2 x^4 + 3 \Omega_1^6 \right]^{1/2}, \qquad (9)$$

$$C = \left[\frac{1}{9}D^2 + \frac{1}{3}\Omega_1^2 + \frac{1}{3}x^2\right]^{1/2},\tag{10}$$

$$\theta = \arccos\left(A/C^3\right),\tag{11}$$

and

$$A = -\frac{1}{27}D^3 + \frac{1}{3}Dx^2 - \frac{1}{6}D\Omega_1^2.$$
 (12)

However, it is clear that if we try to treat exactly the multispin correlation presented in equations (2-4), the problem is mathematically intractable. Therefore, we shall take a decoupling approximation [12,13]

$$\langle \sigma_i^z \sigma_j^z ... \sigma_l^z \rangle \approx \langle \sigma_i^z \rangle \langle \sigma_j^z \rangle ... \langle \sigma_l^z \rangle,$$
 (13)

$$\langle S_i^z (S_j^z)^2 ... S_l^z \rangle \approx \langle S_i^z \rangle \langle (S_j^z)^2 \rangle ... \langle S_l^z \rangle,$$
 (14)

for $i \neq j \neq ... \neq l$. By applying the approximation, the averaged A sublattice magnetization σ , B sublattice magnetization m, and quadrupolar moment q can be evaluated from the following coupled equations:

$$\sigma = \langle \sigma_i^z \rangle = \left[q \cosh \left(J \nabla \right) + m \sinh \left(J \nabla \right) + 1 - q \right]^4 F(x) \Big|_{x=0}, \tag{15}$$

$$m = \left\langle S_j^z \right\rangle = \left[\cosh\left(\frac{J}{2}\nabla\right) + 2\sigma \sinh\left(\frac{J}{2}\nabla\right) \right]^4 G(x) \Big|_{x=0},$$
(16)

$$q = \left\langle \left(S_j^z\right)^2 \right\rangle = \left[\cosh\left(\frac{J}{2}\nabla\right) + 2\sigma\sinh\left(\frac{J}{2}\nabla\right)\right]^4 H(x)\Big|_{x=0}.$$
(17)

In the vicinity of the second order phase transition line, we may expand the right hand sides of equations (15-17) with respect to σ , m, and q. The set of coupled equations is then:

$$\sigma = 4(K_1q^3 + 3K_2q^2(1-q) + 3K_3q(1-q)^2 + K_4(1-q)^3)m + 4(K_5q + K_6(1-q))m^3, \quad (18)$$

$$m = 8L_1\sigma + 32L_2\sigma^3, (19)$$

$$q = Q_1 + 24Q_2\sigma^2 + 16Q_3\sigma^4.$$
⁽²⁰⁾

In order to obtain the A sublattice magnetization σ , we have to combine equations (18-20). Then the selfconsistent equation of the A sublattice magnetization σ is given

$$\sigma = a\sigma + b\sigma^3 + \dots \tag{21}$$

where

$$a = 32L_1 \left[K_1 Q_1^3 + 3K_2 Q_1^2 (1 - Q_1) + 3K_3 Q_1 (1 - Q_1)^2 + K_4 (1 - Q_1)^3 \right]$$
(22)

$$b = 128L_{2} [K_{1}Q_{1}^{3} + 3K_{2}Q_{1}^{2}(1 - Q_{1}) + 3K_{3}Q_{1}(1 - Q_{1})^{2} + K_{4}(1 - Q_{1})^{3}] + 2048L_{1}^{3} [K_{5}Q_{1} + K_{6}(1 - Q_{1})] + 576L_{1}Q_{2} [K_{1}Q_{1}^{2} + K_{2}Q_{1}(2 - 3Q_{1}) + K_{3}(1 - Q_{1})(1 - 3Q_{1}) - K_{4}(1 - Q_{1})^{2}].$$
(23)

The coefficients of the above equations (22, 23) are lengthy expressions given in the appendix. Since σ is small enough near the second phase transition line, we retain only first order and second order terms to be able to get an explicit solution for the A sublattice magnetization. Then the A sublattice magnetization σ can be given by

$$\sigma^2 = (1 - a)/b.$$
(24)

The second order phase transition line is determined by the following equation:

$$a = 1 \quad \text{and} \quad b < 0. \tag{25}$$

The right hand side of equation (24) must be positive. If this is not the case, the transition is of the first order, and hence the point at which a = 1 and b = 0 is the tricritical point. It should be noted here that in the above discussions we have not touched on the sign of J. When Jis positive, the ground state of the mixed Ising system is ferromagnetic. On the other hand, when J is negative, the system is ferrimagnetic. In the present system sublattices A and B have different transverse fields, from both the theoretical and experimental point of view the study may be very significant.

3 Numerical results and discussions

In this section, we would like to study the influence of the different transverse fields on the tricritical point and reentrant phenomena of the mixed different transverse Ising spin system with single-ion anisotropy on the square lattice. By solving equation (25) numerically, we can obtain the second phase transition line of the present system.

Figures 1a, 1b, 1c express the dependence of the Curie temperature on the single-ion anisotropy parameter for three cases corresponding to the transverse field values of the A sublattice $\Omega_{1/2}/J = 0.0, 0.552$ and 1.4, respectively, when the transverse field value Ω_1/J of the B sublattice is changed. For square lattice (z = 4), there is a possibility of the existence, under certain conditions, of a tricritical point at which the transition changes from second order to first. The full circles denote the tricritical points. As is seen from Figure 1a, when the value of D/J takes a large negative value, on the curve labeled $\Omega_1/J = 0.0$ the tricritical point appears. Moreover, the transition temperature is given by $k_{\rm B}T_{\rm c}/J = 1.2988$ in zero single-ion anisotropy parameter, which is to be compared with the results of the standard mean field approximation $(k_{\rm B}T_{\rm c}/J = 1.633)$ [8], the Bethe-Peierls method $(k_{\rm B}T_{\rm c}/J = 1.240)$ [10] and the finite cluster approximation $(k_{\rm B}T_{\rm c}/J = 1.298)$ [14]. This behaviour is in good agreement with that of the Blume-Capel model [12]. Obviously, the present result is quite superior to that of the standard mean field approximation, slightly different from that of the Bethe-Peierls method and consistent with that of the finite cluster approximation. The decoupling approximation in the present system does not affect the result qualitatively from a comparison with the above-mentioned in some known works. Hence, the decoupling approximation may be a simple but valid method. On the other hand, the transverse field makes the transition temperature decrease; therefore, at a certain value of Ω_1/J , the tricritical point may disappear. We calculate the possibility of the existence of the tricritical point. From our detailed numerical investigations, we have found that the present system exhibits tricritical points for $0 \leq \Omega_1/J < 0.5876$. When $\Omega_1/J \geq 0.5876$, the tricritical point does not appear in the present system (see curves $\Omega_1/J = 0.5876; 1.0; 2.0$). From Figure 1b we can see that if $\Omega_{1/2}/J = 0.5520$, *i.e.*, the transverse field value of the A sublattice is small, and the phase diagram is similar to that in the Figure 1a case. However, it should be noted here that in the case of Figure 1b,



Fig. 1. Curie temperature dependencies of the negative single-ion anisotropy parameter D/J for the A sublattice $\Omega_{1/2}/J$ values of (a) 0.0, (b) 0.5520 and (c) 1.4. The numbers on the curves are the values of Ω_1/J .



Fig. 2. Curie temperature dependencies of the negative single-ion anisotropy parameter D/J for the B sublattice Ω_1/J values of (a) 0.0 and (b) 0.4. The numbers on the curves are the values of $\Omega_{1/2}/J$.



Fig. 3. The scope of the tricritical point that can exist is shown in $(\Omega_{1/2}/J - \Omega_1/J)$ space.

the tricritical point still appears but the system exhibits the tricritical point only for $0 \leq \Omega_1/J < 0.5520$, due to the existence of the A sublattice transverse field. In particular, we notice that the tricritical point just disappears in the present system when $\Omega_{1/2}/J = \Omega_1/J = 0.5520$, *i.e.*, the different transverse fields turn into the uniform transverse field. The result obtained here is consistent with the result in reference [21]. In Figure 1c we assume the A sublattice transverse field to be $\Omega_{1/2}/J = 1.4$, Reentrant phenomena is shown in curves labeled $\Omega_1/J = 0.0$ and 0.4, from which one can see that the reentrant phenomenon is depressed with increasing B sublattice transverse field Ω_1/J . In other words, when the $\Omega_{1/2}/J$ is large and the Ω_1/J is not too large, the reentrant phenomenon becomes weak. When the Ω_1/J is larger than this certain value the reentrant phenomenon vanishes. Hence, the role of the B sublattice transverse field Ω_1/J is to destroy the reentrant phenomenon. We may also determine that in this case the system exhibits a tricritical point for $0 \leq \Omega_1/J < 0.4426$. On the other hand, we can observe a characteristic phenomenon in Figures 1a and 1b. That is, with increasing the value of the B sublattice transverse field Ω_1/J , the negative single-ion anisotropy parameter first increases and then decreases. We also note that with increasing the value of the A sublattice transverse field $\Omega_{1/2}/J$, the phenomenon gradually becomes weak and then disappears. The phenomenon cannot be obtained by using the mixed uniform transverse Ising spin system [21].

In Figures 2a and 2b, we plot the dependence of the Curie temperature on the single-ion anisotropy for the present system with $\Omega_1/J = 0.0$ and 0.4, respectively, when the value of $\Omega_{1/2}/J$ is changed. As is seen from Figure 2a, the second order transition temperature goes to zero at a value of D/J = -1.0 if the value of the A sublattice transverse field varies in the ranges $2.193 \leq \Omega_{1/2}/J \leq 5.267$, while the tricritical point appears in the $0.0 \leq \Omega_{1/2}/J \leq 2.192$ region. In other words, the second order transition does not exist in the low temperature region when $\Omega_{1/2}/J$ is not too large; the second

order transition could appear at zero temperature but, when $\Omega_{1/2}/J$ is larger. Therefore, the existence or disappearance of the tricritical point depends on the critical value $\Omega_{1/2}/J = 2.193$. It is obvious that the tricritical temperature and tricritical negative single-ion anisotropy parameter decreases monotonically with increasing the $\Omega_{1/2}/J$. On the other hand, for $\Omega_{1/2}/J = 1.0, 1.8, 2.2,$ and 3.0, the reentrant phenomenon can be observed. However, for $\Omega_{1/2}/J = 0.0, 0.5, 3.8$, and 4.6, the reentrant phenomenon is not observed. In this way, when the value of the A sublattice transverse field varies in the ranges $0.793 \leq \Omega_{1/2}/J \leq 3.473$, the phase transition line may exhibit reentrant phenomena in the (T, D) space. It is important to notice that the second order reentrant phenomenon occurs with increased $\Omega_{1/2}/J$. Here the role of $\Omega_{1/2}/J$ is not to destroy but to assist the reentrant phenomenon. Figure 2b shows that, as compared to the previous case of Figure 2a, values of the negative singleion anisotropy parameter D/J for which the second order transition temperature goes to zero are no longer the same for different values of $\Omega_{1/2}/J$. In this case, the reentrant phenomenon can also be observed under $\Omega_1/J = 0.4$ (see the curves labelled 1.5 and 2.0), but the reentrant phenomenon is depressed. This behaviour of the different transverse fields $\Omega_{1/2}/J$ and Ω_1/J can be seen from a comparison between Figures 2a and 2b. This means that the A sublattice transverse field $\Omega_{1/2}/J$, under certain ranges, will assist the occurrence of the reentrant phenomenon, while the B sublattice transverse field Ω_1/J will destroy the reentrant phenomenon. Thus, the influence of the $\Omega_{1/2}/J$ and Ω_1/J on the reentrant phenomenon is very different.

In Figure 3 the localization of the tricritical point in the $(\Omega_1/J, \Omega_{1/2}/J)$ space is depicted. Clearly, the existence of the tricritical point is affected by the transverse fields $\Omega_{1/2}/J$ and Ω_1/J beside negative single-ion anisotropy parameter. Hence, there may be two different critical sublattice transverse fields values $\Omega_{1/2k}/J$ and Ω_{1k}/J . When $\Omega_{1/2}/J \ge \Omega_{1/2k}/J$ or $\Omega_1/J \ge \dot{\Omega}_{1k}/J$, the tricritical point is no longer obtained. From our calculation, $\Omega_{1/2k}/J = 2.192$ and $\Omega_{1k}/J = 0.5876$. As shown in Figure 3, the existence scope of the tricritical point can be indicated in the present system, if the A sublattice transverse field varies in the ranges $0.0 \leq \Omega_{1/2}/J < 2.192$ and the B sublattice transverse field is in a restricted region $0.0 \leq \Omega_1/J < 0.5876$. In other words, when $\Omega_{1/2}/J \ge 2.192$ or $\Omega_1/J \ge 0.5876$, the tricritical point do not appear in the present system.

Finally, let us discuss the differences between the mixed uniform transverse spin system results and the present results. These differences can be understood by the simple physical interpretation. An important factor follows from the fact of the different transverse fields of both A and B sublattices. Thus the situation entirely differs from the mixed uniform transverse spin system. In particular, considering the uniform transverse field in reference [21], we cannot obtain the reentrant phenomenon and the characteristic phenomenon of the negative single-ion anisotropy parameter in Figures 1a and 1b. Clearly,

two different transverse fields indicate different quantum effects; this leads to the outstanding features of the present system. It is expected to be suitable for more general situation.

4 Conclusion

In this paper, the tricritical point and the reentrant phenomenon have been computed for the mixed different transverse Ising spin system with single-ion anisotropy by means of the effective field theory with correlations, making use of a decoupling approximation. We have discussed in detail the tricritical point and the influence of the different sublattice transverse fields on the tricritical point. We have observed that the present system with the A sublattice transverse field $\Omega_{1/2}/J$ in the ranges $0.0 \leq \Omega_{1/2}/J \leq 2.192$ and the B sublattice transverse field Ω_1/J in the region $0.0 \leq \Omega_1/J \leq 0.5876$ may display tricritical behaviour when the negative single-ion anisotropy parameter takes large values. Furthermore, the characteristic behaviour of the single-ion anisotropy has been discovered by changing the values of the different transverse fields, as depicted in Figures 1a and 1b.

On the other hand, we have shown the existence of the reentrant phenomenon in the present system. Moreover, we have clarified that the different sublattice transverse fields play an opposite role: one induces, the other depresses the reentrant phase transition. That is, the role of the A sublattice transverse field $\Omega_{1/2}/J$ will promote the tendency of the reentrant phenomenon under certain conditions, while the role of the B sublattice transverse field Ω_1/J will destroy the reentrant tendency. This behaviour is explicitly shown in Figures 2a and 2b.

As discussed in Section 3, a number of interesting phenomena have been found, which can be attributed to the competition between the different sublattice transverse fields and the single-ion anisotropy in the present system. Finally, it is important to mention that the results are obtained within the present framework. It is clear that different results would be given if some other approximation methods were adopted [8,10]. However, we believe that the results obtained here are significant for material science.

Appendix

$$K_{1} = \sinh (J\nabla) \left[\cosh (J\nabla) \right]^{3} F(x) \big|_{x=0}$$

$$K_{2} = \sinh (J\nabla) \left[\cosh (J\nabla) \right]^{2} F(x) \big|_{x=0}$$

$$K_{3} = \sinh (J\nabla) \cosh (J\nabla) F(x) \big|_{x=0}$$

$$K_{4} = \sinh (J\nabla)F(x)\big|_{x=0}$$

$$K_{5} = \left[\sinh (J\nabla)\right]^{3} \cosh (J\nabla)F(x)\big|_{x=0}$$

$$K_{6} = \left[\sinh (J\nabla)\right]^{3}F(x)\big|_{x=0}$$

$$L_{1} = \sinh \left(\frac{J}{2}\nabla\right)\left[\cosh \left(\frac{J}{2}\nabla\right)\right]^{3}G(x)\big|_{x=0}$$

$$L_{2} = \left[\sinh \left(\frac{J}{2}\nabla\right)\right]^{3}\cosh \left(\frac{J}{2}\nabla\right)G(x)\big|_{x=0}$$

$$Q_{1} = \left[\cosh \left(\frac{J}{2}\nabla\right)\right]^{4}H(x)\big|_{x=0}$$

$$Q_{2} = \left[\sinh \left(\frac{J}{2}\nabla\right)\right]^{2}\left[\cosh \left(\frac{J}{2}\nabla\right)\right]^{2}H(x)\big|_{x=0}$$

$$Q_{3} = \left[\sinh \left(\frac{J}{2}\nabla\right)\right]^{4}H(x)\big|_{x=0}.$$

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