Transverse-random-field mixed Ising model with arbitrary spins

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The transverse-random-field mixed Ising model consisting of arbitrary spin values has been studied by combining the pair model approximation with discretized path-integral representation. The phase diagrams of systems with mixed spins: $\sigma=1/2$, $S=1$; $\sigma=1/2$, $S=3/2$, and $\sigma=1$, $S=2$ are plotted. Not only the discontinuity at $T=0$ K is found between the trimodal and bimodal distributions of transverse fields, which is similar to the single-spin counterpart, but also the tricritical behavior is observed in these phase diagrams when both transverse fields are trimodal distributed, which is different from the single-spin one. The appearance of tricritical point is independent of the coordination number and spin values.

I. INTRODUCTION

In last decades, there has been an interesting number of works dealing with critical behavior of quantum spin system. The transverse Ising model is the simplest quantum system and has been introduced to explain the phase transition of hydrogen-bonded ferroelectrics such as KH_2PO_4 (Ref. 1) and other systems[2] in the order-disorder phenomenon with tunneling effects. The quantum effect is represented by adding a term (transverse field part) in the Hamiltonian, which is noncommutative with the interaction part. As the transverse field is taken as fixed values, the transverse Ising model has a finite-temperature phase transition which can be depressed to zero temperature at a critical value of the transverse field.[3] As the transverse field is randomly distributed, the phase diagram of single-spin transverse-random-field Ising model has been studied[4,5] and a finite discontinuity in the phase diagram was found at $T=0$ K, between the trimodal and bimodal distributions of the transverse field. Subsequently, Yokota[6] pointed out that the directional randomness of the transverse field did not change the critical behavior.

On the other hand, much attention has been directed to the two-sublattice mixed-spin systems over the years. The mixed-spin Ising model consisting of spin-1/2 and spin-S with a crystal-field interaction has been studied extensively by a variety of techniques, namely the exact,[7,8] and approximated methods[9–13] as well as the high-temperature series expansion method.[14] The tricritical point is predicted in the systems of $S=1$ or 2 with a coordination number z larger than $z=3$.[12,15] However, the tricritical behavior does not exist in the system with $S=3/2$.[16] These results indicate that the existence of tricritical behavior in the mixed-spin Ising model with a crystal-field interaction is dependent on the spin value S as well as the coordination number.

The transverse mixed Ising model has been studied by effective-field theory (EFT),[17] mean-field approximation (MFA),[18] and real-space renormalization-group approximation (RSRGA).[19] These approaches showed that the transition temperature falls to zero at a certain transverse field. But, to our knowledge, no investigation has been made of transverse-random-field mixed Ising model (TRMIM). As a matter of fact, the random distribution of transverse field reveals coexistence of disorder with quantum effect in TRMIM. These two effects operate in different manner when the temperature decreases. Furthermore, since the mixed-spin system has less translational symmetry than the single-spin counterpart, the competition between these two effects may result in many new phenomena in the TRMIM which cannot be observed in the single-spin transverse random-field Ising model or in the transverse mixed Ising model. The aim of this work is to study the phase diagram of the TRMIM when both of the transverse fields are trimodal distributed.

The pair model approximation[20] is one of the usual methods to deal with the mixed-spin Ising model. Under pair model approximation, the Hamiltonian of a nearest-neighbor two-site cluster which is arbitrarily picked up is represented as that of the whole system, where the interaction between these two nearest-neighbor sites is included exactly and the interaction from other sites is approximately considered by mean field. On the other hand, since the transverse-random-field mixed Ising model is a quantum spin system, it is difficult to diagnolize the Hamiltonian directly due to its noncommutativity. Fortunately the discretized path-integral representation[21,22] (DPIR) enables us to analytically obtain the formula of the partition function, the magnetization and so on. Therefore, in this paper we combine these two approaches to deal with TRMIM and to show the magnetization and the equation of the second-order phase transition analytically, and then numerically solve the second-order phase transition equation to plot the phase diagram.

II. THEORY

The Hamiltonian of transverse-random-field mixed Ising model (TRMIM) is given by

$$H=-\sum_{i,j} J\hat{\sigma}_i^z\hat{S}_j^z-\sum_i \Gamma_i\hat{\sigma}_i^x-\sum_j \Gamma_j\hat{S}_j^x. \qquad (1)$$

This model describes the mixed-spin system consisting of two sublattices A and B, which are arranged alternately. In the underlying lattice the sites of A sublattice are occupied by spins $\hat{\sigma}_i$ of magnitude σ, while those of the alternate B sublattice are occupied by spins $\hat{S}_j$ of magnitude S. The $\hat{\sigma}_i$

takes the $2\sigma+1$ values: $-\sigma$, $-(\sigma-1)$, $\ldots$, $(\sigma-1)$, σ and the $\hat{S}_j$ the $2S+1$ values: $-S$, $-(S-1)$, $\ldots$, $(S-1)$, S, where σ and S have one of the usual integer or odd half-integer values. The first summation in Eq. (1) involves all pairs of nearest-neighbor sites in the lattice. The second and third summations involve all sites of A and B, respectively. The quantities, J, Γ_i, and Γ_j, measured in unit of K_BT with K_B the Boltzmann constant and T the temperature, are, respectively, an interaction constant and the transverse fields on the A and B sublattices.

The transverse fields are randomly distributed according to following trimodal distributions:

$$P_1(\Gamma_i)=p_1\delta(\Gamma_i)+\frac{1}{2}(1-p_1)[\delta(\Gamma_i+\Gamma_1)+\delta(\Gamma_i-\Gamma_1)], \tag{2}$$

$$P_2(\Gamma_j)=p_2\delta(\Gamma_j)+\frac{1}{2}(1-p_2)[\delta(\Gamma_j+\Gamma_2)+\delta(\Gamma_j-\Gamma_2)], \tag{3}$$

where the parameters p_1 and p_2 are probabilities of spins $\hat{\sigma}_i$ and $\hat{S}_j$ not exposed to the transverse fields and $0\leqslant p_1,p_2\leqslant 1$. Γ_1 and Γ_2 represents the uniform transverse fields on A and B sublattices. p_1(or p_2)$\neq 0$ means that the transverse field Γ_1(or Γ_2) is trimodal distributed, while p_1(or p_2)$=0$ means that Γ_1(or Γ_2) is bimodal distributed.

Within the pair model approximation, the Hamiltonian (1) may be rewritten as

$$H_p=-J\hat{\sigma}_i^z\hat{S}_j^z-\Gamma_i\hat{\sigma}_i^x-\Gamma_j\hat{S}_j^x-A\hat{\sigma}_i^z-B\hat{S}_j^z, \tag{4}$$

with

$$A=J(z-1)m_2,\quad B=J(z-1)m_1, \tag{5}$$

where z is the coordination number, m_1 and m_2 are the average magnetizations of spin-σ and spin-S, respectively.

Due to the noncommutative operators in the Hamiltonian H_p, it is very difficult to derive the eigenvalues of it. In order to solve this problem, we shall reformulate the Hamiltonian under the discretized path-integral representation (DPIR) to obtain the spin-pair partition function. In DPIR, the quantized (2S+1)-states spin on each site will be transferred into P-component vector $U(U^{(1)}, U^{(2)}, \ldots, U^{(P)})$ and eventually to let P go to infinity. Each component $U^{(t)}=S$, $(S-1)$, $\ldots$, $-(S-1)$, $-S$ and the net effect is to represent the quantum uncertainty by creating many copies, or replicas of the original variables. By means of the DPIR, the pair Hamiltonian can be broken up into two reference parts involving only the single-site term, and an interaction part. The corresponding free energy can be expressed in terms of the free energy of the reference parts and a cumulant expansion. By taking the first cumulant term, the expression of the partition function of the spin pair reads as

$$\ln Q_p=\ln Q_\sigma^1+\ln Q_S^1+\frac{J}{\beta}\frac{\partial}{\partial A}[\ln Q_\sigma^1]\frac{\partial}{\partial B}[\ln Q_S^1], \tag{6}$$

where Q_σ^1 and Q_S^1 are the one-body partition functions of spin-σ and spin-S, respectively,

$$Q_\sigma^1=\exp[-\beta H_\sigma^1], \tag{7}$$

$$Q_S^1=\exp[-\beta H_S^1], \tag{8}$$

with

$$H_\sigma^1=-\Gamma_i\hat{\sigma}_i^x-A\hat{\sigma}_i^z, \tag{9}$$

$$H_S^1=-\Gamma_j\hat{S}_j^x-B\hat{S}_j^z. \tag{10}$$

The average values of spin-σ and spin-S may be given as

$$\langle\sigma^z\rangle=\frac{1}{\beta}\frac{\partial}{\partial A}(\ln Q_p), \tag{11}$$

$$\langle S^z\rangle=\frac{1}{\beta}\frac{\partial}{\partial B}(\ln Q_p). \tag{12}$$

Since the transverse fields are randomly distributed according to trimodal random distributions, the average magnetizations of spin-σ and spin-S should be obtained by averaging over the probability distributions of the transverse fields, thus

$$m_1=\int\int d\Gamma_i d\Gamma_j\langle\sigma^z\rangle P_1(\Gamma_i)P_2(\Gamma_j), \tag{13}$$

$$m_2=\int\int d\Gamma_i d\Gamma_j\langle S^z\rangle P_1(\Gamma_i)P_2(\Gamma_j). \tag{14}$$

In the vicinity of the transition temperature, the magnetizations m_1 and m_2 tend to zero, we may expand the right-hand side of Eqs. (13) and (14) with respect to m_1 and m_2 and retain only terms linear to m_1 and m_2,

$$m_1=a_1A+b_1B, \tag{15}$$

$$m_2=a_2A+b_2B, \tag{16}$$

where a_1, a_2, b_1, and b_2 are functions of p_1, p_2, Γ_1, and Γ_2 and their expressions depend on the values of spin-σ and spin-S,

$$a_1=p_1\frac{\Sigma_{\sigma'}\sigma'^2}{2\sigma'+1}+(1-p_1)\frac{\Sigma_{\sigma'}\sigma'\exp(\sigma'\Gamma_1)/\Gamma_1}{\Sigma_{\sigma'}\exp(\sigma'\Gamma_1)}, \tag{17}$$

$$b_1=\beta J\left[p_1\frac{\Sigma_{\sigma'}\sigma'^2}{2\sigma'+1}+(1-p_1)\frac{\Sigma_{\sigma'}\sigma'\exp(\sigma'\Gamma_1)/\Gamma_1}{\Sigma_{\sigma'}\exp(\sigma'\Gamma_1)}\right]$$
$$\times\left[p_2\frac{\Sigma_{S'}S'^2}{2S'+1}+(1-p_2)\frac{\Sigma_{S'}S'\exp(S'\Gamma_2)/\Gamma_2}{\Sigma_{S'}\exp(S'\Gamma_2)}\right], \tag{18}$$

$$a_2=b_1, \tag{19}$$

$$b_2=p_2\frac{\Sigma_{S'}S'^2}{2S'+1}+(1-p_2)\frac{\Sigma_{S'}S'\exp(S'\Gamma_2)/\Gamma_2}{\Sigma_{S'}\exp(S'\Gamma_2)}, \tag{20}$$

where S' takes (2S+1) values: $-S$, $-(S-1)$, $\ldots$, $(S-1)$, S, and σ' takes $(2\sigma+1)$ values: $-\sigma$, $-(\sigma-1)$, $\ldots$, $(\sigma-1)$, σ. Then the second-order phase transition line is determined by the following equation:

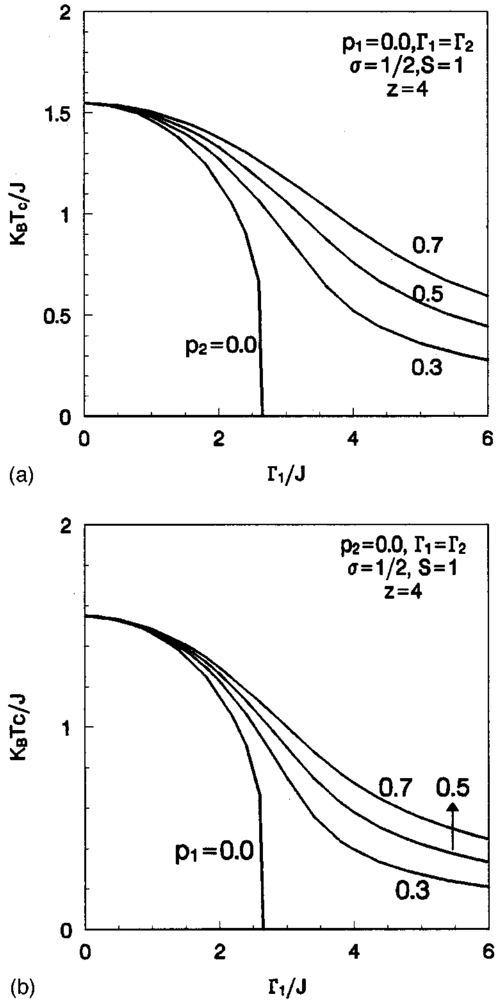

FIG. 1. Reduced transition temperature K_BT_c/J of system $\sigma=1/2$ and $S=1$ with $z=4$ as a function of the transverse field Γ_1/J in the case of $\Gamma_1=\Gamma_2$ and for (a) $p_1=0.0$ with $p_2=0.0$, 0.3, 0.5, and 0.7; (b) $p_2=0.0$ with $p_1=0.0$, 0.3, 0.5, and 0.7.

$$a_1\times b_2-\left(a_2-\frac{1}{(z-1)\beta J}\right)\times\left(b_1-\frac{1}{(z-1)\beta J}\right)=0. \tag{21}$$

III. CALCULATION AND DISCUSSION

Here we are only interested in the critical behavior of the transverse-random-field mixed Ising model (TRMIM) with transverse fields trimodal distributed, which may be studied by solving Eq. (21) numerically. We take the following systems as samples to show the common feature of the TRMIM: $\sigma=1/2$, $S=1$ with $z=4$; $\sigma=1/2$, $S=3/2$ with $z=3$ and 4, and $\sigma=1$, $S=2$ with $z=4$. The values of transverse fields Γ_i and Γ_j are assumed to be equal in these systems for simplicity, $\Gamma_1=\Gamma_2$, but p_1 may be the same as or different from p_2.

First we consider the TRMIM of $\sigma=1/2$ and $S=1$ with $z=4$. Figure 1(a) shows the reduced critical temperature as a function of Γ_1/J in the case of $p_1=0.0$ with $p_2=0.0$, 0.3, 0.5, and 0.7, respectively. In this case the transverse field of $\sigma=1/2$ is bimodal distributed and the transverse field of $S=1$ is bimodal ($p_2=0.0$) or trimodal ($p_2\neq 0.0$) distributed.

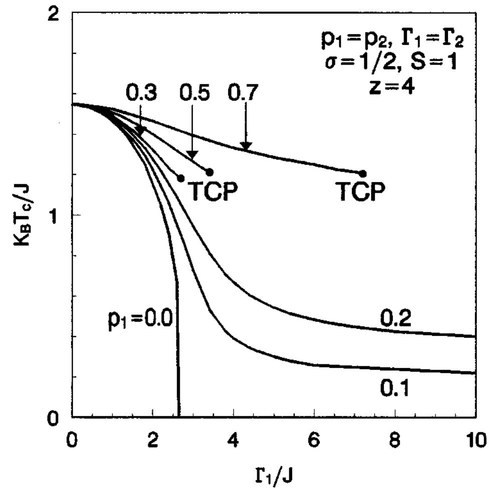

FIG. 2. The change of K_BT_c/J of system $\sigma=1/2$ and $S=1$ with $z=4$ with the transverse field Γ_1/J in the case of $\Gamma_1=\Gamma_2$ for $p_1=p_2=0.0$, 0.1, 0.2, 0.3, 0.5, and 0.7. The solid circles refer to the tricritical points (TCP).

As $p_1=p_2=0.0$, the transition temperature decreases rapidly with increasing the transverse field and the transition temperature reaches zero at $\Gamma_1/J=2.65$. This behavior is in good agreement with that of transverse mixed Ising model.[17–19] In particular, the value of the temperature at $\Gamma_1/J=0.0$ is 1.52, which may be comparable with the EFT result[17] 1.30, the RSRGA result[19] 1.37, and the MFA result[18] 1.63. The value of critical transverse field is 2.65, which is comparable with the EFT result[17] 2.12 and the MFA result[18] 2.83. These results illustrate that the pair model approximation with the DPIR is suitable to study the TRMIM and is superior to the mean-field approximation. When p_2 is larger than zero, the transition temperature falls with increasing transverse field but cannot reach zero no matter how large the transverse fields are. The increment of p_2 leads to the shift of the transition temperature at the same transverse field.

When Γ_2 is bimodal ($p_2=0.0$) and Γ_1 is bimodal ($p_1=0.0$) or trimodal ($p_1\neq 0.0$) distributed, the phase diagram is potted in Fig. 1(b). Similarly the temperature reaches zero only when the transverse field Γ_1 is bimodal distributed. The temperatures of $p_2=0.0$ and $p_1=0.3,0.5,0.7$ in Fig. 1(b) are lower than corresponding to those of $p_1=0.0$ and $p_2=0.3,0.5,0.7$ in Fig. 1(a) at the same transverse field. From Figs. 1(a) and 1(b), one may conclude that the critical behavior of TRMIM with bimodal distributions of the transverse fields is the same as that of transverse mixed Ising model, where the temperature monotonously falls to zero at critical transverse field. But the trimodal distribution of one of transverse field leads to the transition temperature to be nonzero, that is, disappearance of the critical transverse field.

Next we study the phase diagram with both p_1 and p_2 being nonzero values. In Fig. 2, the change of transition temperature with Γ_1 is potted with $p_1=p_2=0.0$, 0.1, 0.2, 0.3, 0.5, and 0.7. The situation of $p_1=p_2=0.0$ has been discussed in Fig. 1. As p_1+p_2 is small ($p_1=p_2=0.1$, 0.2), the temperature continuously decreases with increasing Γ_1 but cannot reach zero. When p_1+p_2 is

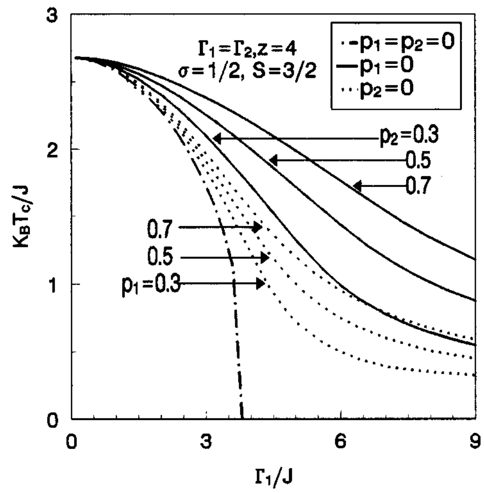

FIG. 3. K_BT_c/J of system $\sigma=1/2$ and $S=3/2$ with $z=4$ vs Γ_1/J in the case of $\Gamma_1=\Gamma_2$ and for $p_1=p_2=0.0$ (dot-dashed line), for $p_1=0.0$ with $p_2=0.3$, 0.5, 0.7 (solid lines) and for $p_2=0.0$ with $p_1=0.3$, 0.5, 0.7 (dotted lines).

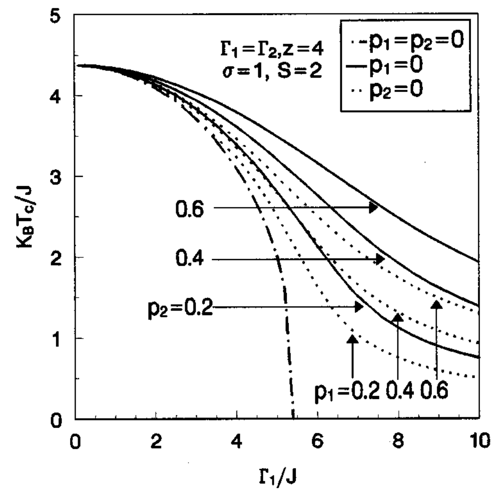

FIG. 5. K_BT_c/J of system $\sigma=1$ and $S=2$ with $z=4$ vs Γ_1/J in the case of $\Gamma_1=\Gamma_2$ and for $p_1=p_2=0.0$ (dot-dashed line), for $p_1=0.0$ with $p_2=0.2$, 0.4, 0.6 (solid line) and for $p_2=0.0$ with $p_1=0.2$, 0.4, and 0.6 (dotted lines).

large enough ($p_1=p_2=0.3$, 0.5, and 0.7), the temperature falls initially but then terminates at a finite value. This behavior is called tricritical behavior and the terminal point is named as tricritical point (TCP, the solid circles in figure). The temperature of the tricritical point is around $K_BT_c/J=1.20$. However the transverse field of tricritical point becomes larger with increasing the value of p_1+p_2.

As we know, the transverse field gives rise to a possible spin-flip transition and hence induces the quantum fluctuation. Nevertheless, the trimodal distribution of the transverse field reflects a form of disorder which coexists with the quantum effect in TRMIM. They behave in a different manner as the temperature is depressed. The case that one of the transverse field is bimodal distributed and the other is trimodal distributed in TRMIM is similar to that of trimodal distribution of transverse field in single-spin transverse-random-field Ising model. The phase diagram of this case shows the discontinuity which has been discussed in Refs. 4–6. As both of the transverse fields are trimodal distributed, the effect of quantum fluctuation is relatively weakened. At small value of p_1+p_2, the quantum effect still dominates, and the disorder from the random distribution only leads to the nonzero temperature. With increasing the value of p_1+p_2, the disorder effect may match and eventually overpass the quantum effect. In addition, the mixed-spin system has less translational symmetry than the single-spin one. These two effects in TRMIM result in the appearance of the tricritical point. With further increasing p_1 and p_2, the transverse field has to be increased to compete the disorder effect.

In mixed-spin Ising model with crystal field,[16] the phase diagram of system $\sigma=1/2$ and $S=3/2$ is different from that of system $\sigma=1/2$ and $S=1$, where the tricritical point does

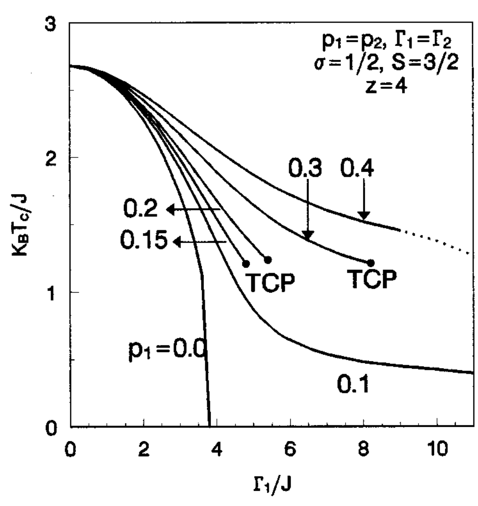

FIG. 4. K_BT_c/J of system $\sigma=1/2$ and $S=3/2$ with $z=4$ vs Γ_1/J in the case of $\Gamma_1=\Gamma_2$ for $p_1=p_2=0.0$, 0.1, 0.15, 0.2, 0.3, and 0.4. The solid circles refer to the tricritical points (TCP).

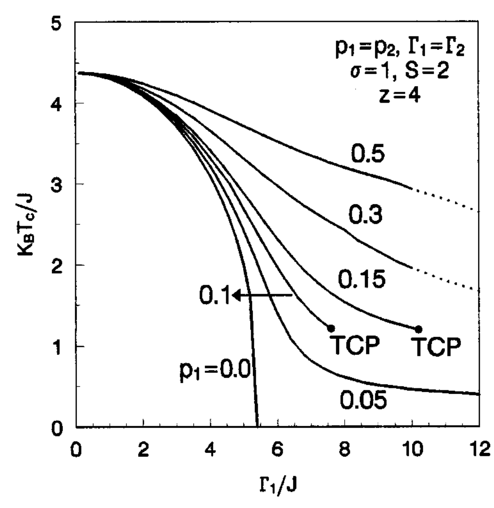

FIG. 6. K_BT_c/J of system $\sigma=1$ and $S=2$ with $z=4$ vs Γ_1/J in the case of $\Gamma_1=\Gamma_2$ for $p_1=p_2=0.0$, 0.05, 0.1, 0.15, 0.3, and 0.4. The solid circles refer to the tricritical points (TCP).

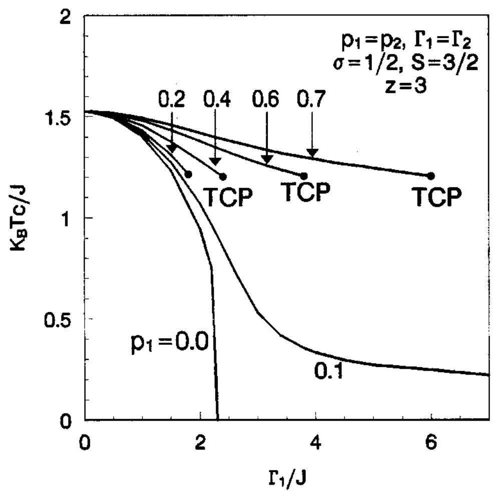

FIG. 7. K_BT_c/J of system $\sigma=1/2$ and $S=3/2$ with $z=3$ vs Γ_1/J in the case of $\Gamma_1=\Gamma_2$ for $p_1=p_2=0.0$, 0.1, 0.2, 0.4, 0.6, and 0.7. The solid circles refer to the tricritical points (TCP).

not exist. Does the tricritical point exist in TRMIM of $\sigma=1/2$ and $S=3/2$ or not? Figure 3 shows K_BT_c/J vs Γ_1/J in three cases: $p_1=p_2=0.0$ (dot-dashed line); $p_1=0.0$, $p_2\neq 0.0$ (solid lines), and $p_2=0.0$, $p_1\neq 0.0$ (dotted lines). In this phase diagram, the trimodal distribution of one of the transverse fields similarly leads to the discontinuity of phase diagram at $T=0$ K but the directional randomness (bimodal distribution) of both transverse fields shows the same phase transition behavior as the fixed transverse field. The transition temperature in the case of $p_1=0.0$ is higher than that in the case of $p_2=0.0$. This demonstrates that the disorder from $S=3/2$ gives rise to more influence on phase transition than that from $\sigma=1/2$. As shown in Fig. 3 the values of critical transverse field, the temperature at the same p_1, p_2 and Γ_1 are higher than those in Fig. 1 because of the increment of spin S from 1 to 3/2.

As p_1 and p_2 are nonzero values, the phase diagram of $\sigma=1/2$ and $S=3/2$ is shown in Fig. 4. In this figure the tricritical point shows up when both p_1 and p_2 are larger than 0.15. The dotted line of curve 0.4 indicates that the transition temperature will decrease with increasing Γ_1 and Γ_2 and eventually terminates at the same temperature as the curves 0.15 and 0.3. The tricritical point of this curve ($p_1=p_2=0.4$) is not drawn in the figure but may be observed at high transverse field. For the system consisting of both odd half-integer spins, the tricritical point may exist but the values of p_1 and p_2, where the tricritical point appears, are less than those of the system of $\sigma=1/2$ and $S=1$.

The phase diagram of systems with odd half-integer spin value have been studied and the tricritical behavior is shown in above figures. How is the phase diagram of system with both integer spins mixed? Figures 5 and 6 show the phase diagrams of system $\sigma=1$ and $S=2$. In Fig. 5, where one of the transverse field is bimodal distributed, the phase diagram exhibits the discontinuity at $T=0$ K as those of systems $\sigma=1/2$, $S=1$ and $\sigma=1/2$, $S=3/2$. In Fig. 6, where both transverse fields are trimodal distributed ($p_1,p_2\neq$ 0.0), the tricritical point shows up when $p_1=p_2$ is larger than 0.1. The tricritical points of curves 0.3 and 0.5 are not drawn in the figure but may be observed as the transverse field is large enough, which are indicated with dotted lines.

From above discussed phase diagrams, we may conclude that the tricritical point may exist in the transverse-random-field mixed Ising model (TRMIM) with integer spin values or odd half-integer spin values. The values of p_1, p_2, Γ_1, and Γ_2, at which the tricritical point appears, are dependent on the spin values. The values of p_1 and p_2 are lowered but those of Γ_1 and Γ_2 are raised with increasing the spin values.

On the other hand, the existence of the tricritical point in mixed-spin Ising model with crystal field is dependent on the coordination number z.[15] Figure 7 shows the phase diagram of system $\sigma=1/2$ and $S=3/2$ with $z=3$. The tricritical points are observed in the curves when the values of both p_1 and p_2 are larger than 0.2. Comparing with Fig. 2, one may see that the critical transverse field, the temperature and the values of p_1 and p_2, Γ_1 and Γ_2 at which the tricritical points appear are lowered because of reduction of interaction in system with $z=3$.

IV. CONCLUSION

In summary, by investigating the phase diagrams of transverse-random-field mixed Ising model (TRMIM): $\sigma=1/2$, $S=1$; $\sigma=1/2$, $S=3/2$, and $\sigma=1$, $S=2$, one may conclude that the bimodal distribution ($p_1=p_2=0$) of the transverse fields in TRMIM results in the same critical behavior as the fixed transverse field in transverse mixed Ising model. The trimodal distribution of transverse field at one of spins ($p_1=0,p_2\neq 0$ or $p_1\neq 0,p_2=0$) only leads to the discontinuity of phase diagram at $T=0$ K, which is similar to the single-spin transverse-random-field Ising model. When both the transverse fields are trimodal distributed ($p_1\neq 0,p_2\neq 0$), not only the discontinuity at small value of p_1+p_2 but the tricritical behavior at large value of p_1+p_2 shows up in the phase diagram. The existence of the tricritical behavior is independent of the spin values and the coordination number. However, the values of p_1, p_2 and transverse fields, Γ_1, Γ_2, at which the tricritical point appears, depend on the spin values and the coordination number.

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