Phase diagrams of the quantum transverse spin- $\frac{3}{2}$ Ising system with bimodal random field

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The bimodal random field quantum spin- $\frac{3}{2}$ Ising system is investigated by combining the pair approximation with the discretized path-integral representation. The second-order phase transition lines, and tricritical points are obtained for the bimodal random field distribution. Reentrant phase transitions, which may be caused by the competition between quantum effects and randomness, are observed. The phase diagrams with respect to the random field and the second-order phase transition temperature, i.e., (H, T) plane, are studied extensively for given values of the transverse field *G* and the coordination number *z*.

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I. INTRODUCTION

Phase transitions and the tricritical behaviors of the random field Ising model were studied extensively some years ago.^{1–3} For the spin- $\frac{1}{2}$ Ising model, Aharony⁴ showed that the bimodal random field distribution leads to a tricritical behavior, while the Gaussian distribution always exhibits a secondorder phase transition. Jaščur and Kaneyoshi⁵ studied the spin- $\frac{3}{2}$ Ising model in a bimodal random field within the framework of the effective-field approximation based on exact spin identities and the differential operator technique, and showed that the system exhibiths a tricritical behavior. Mattis⁶ examined the possibility of a first-order phase transition and the existence of a tricritical point for the trimodal random-field distribution within the mean-field approximation, and concluded that there is no tricritical point for the Gaussian distribution (corresponding to $p = \frac{1}{3}$ in the trimodal random field distribution). Various approximate methods were proposed to improve the results of the mean-field approximation in this model.⁷

The spin- $\frac{1}{2}$ Ising model in the presence of a transverse field, the transverse Ising model, serves for the study of cooperative phenomena (such as reentrance behavior, etc.) and phase transitions in many physical systems.⁸ One of the problems is how the form of the random fields affects the structure of the phase diagrams of the systems represented by the transverse Ising model (TIM). In some of the previous works, the effects of the shapes of a random field on the phase transitions in a quantum transverse spin- $\frac{1}{2}$ Ising model^{9–11} and a spin-1 model¹² are investigated.

The quantum spin system with a random field was investigated by combining the pair approximation with the discretized path-integral representation (DPIR) for spin- $\frac{1}{2}$ (Ref. 11) and for spin-1 models.¹² In these works, the phase diagrams were obtained numerically for some values of the coordination number *z* including $z \rightarrow \infty$, the mean-field approximation (MFA), the existence of tricritical points, and reentrance phenomena were examined for various symmetrical random field distributions. Spin- $\frac{3}{2}$ models were introduced to explain phase transition¹³ in DyVO₄ (Refs. 14 and 15) and tricritical properties in ternary fluid mixtures.¹⁶ These were studied by the mean-field approximation. Recently phase transitions in the spin- $\frac{3}{2}$ Blume-Emery-Griffiths model with nearest-neighbor interaction, both bilinear and biquadratic, and with a crystal-field interaction, were studied within the MFA and the Monte Carlo simulation,¹⁷ and by the renormalization-group method.¹⁸ On the other hand, the quantum spin- $\frac{3}{2}$ Ising model in the presence of both transverse field and random fields was not studied with the present formalism; therefore, it should also be studied extensively, since many cooperative phenomena could only be explained by spin- $\frac{3}{2}$ Ising models.

In this paper, the bimodal random-field quantum spin- $\frac{3}{2}$ Ising model is investigated by combining the pair approximation with the discretized path-integral representation.^{11–12} An analytical expression for the second-order phase transition line is obtained for the bimodal random-field distribution, and the phase diagrams are obtained numerically in the (H, T) plane for various values of the coordination number zand the transverse field G. It is observed that the system exhibits tricritical points, and reentrant phenomena for appropriate ranges of transverse field and bimodal random field are likely due to the competition between the quantum fluctuations and randomness.

The outline of the remainder of the paper is as follows: In Sec. II, the model is introduced, and the analytical expression for the average free energy is obtained. In Sec. III an analytical expression for the second-order phase transition line is obtained, and the existence of tricritical points and the results of the phase diagrams are discussed.

II. HAMILTONIAN AND MODEL

We consider the transverse Ising model with a bimodal random field

$$P(h_i) = \frac{1}{2} \left[\delta(h_i + h_0) + \delta(h_i - h_0) \right].$$
(1)

The Hamiltonian of the model is given by

$$H = -J\sum_{ij} S_i^z S_j^z - \Gamma \sum_i S_i^x - \sum_i h_i S_i^z, \qquad (2)$$

where S_i^z and S_i^x are the quantum spin- $\frac{3}{2}$ operators at site *i*, Γ is the transverse Ising field, and h_i is the random field given by Eq. (1). The quantum spin- $\frac{3}{2}$ operators are given as

$$S_{i}^{z} = \begin{bmatrix} 0 & \sqrt{3}/2 & 0 & 0 \\ \sqrt{3}/2 & 0 & 1 & 0 \\ 0 & 1 & 0 & \sqrt{3}/2 \\ 0 & 0 & \sqrt{3}/2 & 0 \end{bmatrix},$$
$$S_{i}^{z} = \begin{bmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{bmatrix}.$$
(3)

The one-body effective Hamiltonian in the pair approximation is given by

$$H^{(1)} = -\Gamma S_{i}^{x} - (h_{i} + H^{\text{eff}}) S_{i}^{z}, \qquad (4)$$

where H^{eff} is the one-body effective field. The corresponding one-body partition function can be obtained from Eqs. (3) and (4) as

$$Z_i(h_i, H^{\text{eff}}, \Gamma) = 2 \cosh\{\frac{3}{2}\beta \sqrt{[\Gamma^2 + (h_i + H^{\text{eff}})]}\} + 2 \cosh\{\frac{1}{2}\beta \sqrt{[\Gamma^2 + (h_i + H^{\text{eff}})^2]}\}.$$
 (5)

The pair Hamiltonian in the pair approximation is given by

$$H^{(2)} = -JS_i^z S_j^z - (h_i + h^{\text{eff}}) S_i^z - (h_j + h^{\text{eff}}) S_j^z - \Gamma(S_i^x + S_j^x),$$
(6)

where h^{eff} is an effective field, which is related to the onebody effective field H^{eff} by $h^{\text{eff}} = [(z-1)/z]H^{\text{eff}}$. The corresponding pair partition function becomes

$$Z(h_i, h_j, h^{\text{eff}}, \Gamma) = \operatorname{Tr} \exp(-\beta H^{(2)}).$$
(7)

The pair Hamiltonian contains noncommuting operators. In order to eliminate this problem we reformulate the pair Hamiltonian in the DPIR to obtain the pair partition function. In the DPIR, the quantal four-state spin- $\frac{3}{2}$ operator, on each lattice site is converted into a *P*-component vector $U(U^{(1)}, U^{(2)}, ..., U^{(P)})$, and eventually *P* goes to infinity. Each component $U^{(t)}(t=1,2,...,P)$ is then taken to be a classical spin variable $U^{(t)} = \pm \frac{3}{2}$ and $\pm \frac{1}{2}$, 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 a reference part $H_0^{(2)}$, which involves only single-site terms, and an interaction part *V*, which is

$$H^{(2)} = H_0^{(2)} + V, (8)$$

where

$$-\beta H_0^{(2)} = \mathbf{U}_i \cdot \mathbf{a} \cdot \mathbf{U}_i + \mathbf{U}_j \cdot \mathbf{a} \cdot \mathbf{U}_j + \mathbf{h}_i \cdot \mathbf{U}_i + \mathbf{h}_j \cdot \mathbf{U}_j + PC,$$

with

$$(\mathbf{a})_{t,t'} = a \, \delta_{t,t'-1}, \quad (\mathbf{a})_{p,1} = a$$

$$a = \frac{1}{2} \ln \coth\left[\frac{\beta\Gamma}{P}\right], \quad C = \frac{1}{2} \ln\left[\cosh\left[\frac{\beta\Gamma}{P}\right]\sinh\left[\frac{\beta\Gamma}{P}\right]\right],$$
$$\mathbf{h}_{i} = \frac{\beta(h_{i} + h^{\text{eff}})}{P}(1, 1, ..., P)$$

and

$$-\beta V = \frac{\beta J}{P} \mathbf{U}_i \cdot \mathbf{U}_j \,. \tag{9}$$

The free energy can be expressed in terms of the free energy $F_0^{(2)}$ of the reference part and the cumulant expansion in the reference part,

$$-\beta F^{(2)} = \ln \operatorname{Tr} \exp(-\beta H^{(2)})$$
$$= -\beta F_0^{(2)} + \sum_{n=1}^{\infty} \frac{1}{n!} (-\beta)^n C_n(V), \qquad (10)$$

with

$$-\beta F_0^{(2)} = \ln \operatorname{Tr} \exp(-\beta H_0^{(2)}), \qquad (11)$$

and the cumulants are given by

$$C_{1}(V) = \langle V \rangle_{0},$$

$$C_{2}(V) = \langle V^{2} \rangle_{0} - \langle V \rangle_{0}^{2},...,$$
(12)

where $\langle \cdots \rangle_0$ denotes an average over the reference part. We take the first cumulant here; the pair partition function may be evaluated from

$$\ln Z_{ij}(h_i, h_j, h^{\text{eff}}, \Gamma)$$

= ln Tr exp(- $\beta H_0^{(2)}$) - $\beta \langle V \rangle_0$
= ln $Z_i(h_i, h^{\text{eff}}, \Gamma)$ + ln $Z_j(h_j, h^{\text{eff}}, \Gamma)$ + $\beta J m_i m_j$ (13)

where

$$m_i = \beta^{-1} \frac{\partial \ln Z_i(h_i, h^{\text{eff}}, \Gamma)}{\partial h^{\text{eff}}}, \qquad (14)$$

and $Z_i(h_j, h^{\text{eff}}, \Gamma)$ is the same as in Eq. (4), with H^{eff} replaced by h^{eff} .

The free energy $f(h^{\text{eff}})$ in the pair approximation is given by¹⁹

$$-\beta \langle f(h^{\text{eff}}) \rangle_{h} = \langle \ln Z_{i} \rangle_{h} + \frac{z}{2} [\langle \ln Z_{ij} \rangle_{h} - 2 \langle \ln Z_{i} \rangle_{h}], \qquad (15)$$

where $\langle \cdots \rangle_h$ is the average over the random-field distribution, which is bimodal in our case. In order to obtain the free energy $f(h^{\text{eff}})$ explicitly, one needs to calculate m_i from Eq. (14), which is

$$m_{i} = \frac{h_{i} + h^{\text{eff}}}{2\xi} \left[\frac{\sinh\left[\frac{1}{2}\beta\xi\right] + 3\sinh\left[\frac{3}{2}\beta\xi\right]}{\cosh\left[\frac{1}{2}\beta\xi\right] + \cosh\left[\frac{3}{2}\beta\xi\right]} \right], \quad (16)$$

where $\xi = \sqrt{\Gamma^2 + (h_i + h^{\text{eff}})^2}$. Then the explicit form of the free energy is calculated from Eqs. (5), (13), (15), and (16) as

$$-\beta \langle f(h^{\text{eff}}) \rangle_{h} = (1-z) \langle \ln[2 \cosh\{\frac{3}{2}\beta\kappa\} + 2 \cosh\{\frac{1}{2}\beta\kappa\}] \rangle_{h_{i}}$$

$$+ \frac{z}{2} \langle \ln[2 \cosh\{\frac{3}{2}\beta\xi\} + 2 \cosh\{\frac{1}{2}\beta\xi\}] \rangle_{h_{i}}$$

$$+ \frac{z}{2} \langle \ln[2 \cosh\{\frac{3}{2}\beta\xi\} + 2 \cosh\{\frac{1}{2}\beta\xi\}] \rangle_{h_{j}}$$

$$+ \frac{z\beta J}{2} \langle m_{i}m_{j} \rangle_{h_{i},h_{j}}, \qquad (17)$$

where

$$\boldsymbol{\kappa} = \left[\Gamma^2 + \left(h_i + \frac{z}{z-1} h^{\text{eff}} \right)^2 \right]^{1/2},$$

and h_i and h_j means the random field acting on the sites *i* and *j*, respectively.

Now we are in a position ready to calculate the free energy when the system is exposed to bimodal random field distribution; so, using Eq. (1) and taking the average over the bimodal random-field distribution of Eq. (17),

$$-\beta \langle f(h^{\text{eff}}) \rangle = -\frac{z-1}{2} \left[\ln[2\cosh\{\frac{3}{2}\beta\kappa_{+}\} + 2\cosh\{\frac{1}{2}\beta\kappa_{+}\}] + \ln[2\cosh\{\frac{3}{2}\beta\kappa_{-}\} + 2\cosh\{\frac{1}{2}\beta\kappa_{-}\}] \right] + \frac{z}{2} \left[\ln[2\cosh\{\frac{3}{2}\beta\xi_{+}\} + 2\cosh\{\frac{1}{2}\beta\kappa_{-}\}] \right]$$

$$+2\cosh\{\frac{1}{2}\beta\xi_{+}\}] + \ln[2\cosh\{\frac{3}{2}\beta\xi_{-}\} + 2\cosh\{\frac{1}{2}\beta\xi_{-}\}]] + \frac{z\beta J}{8}[(m)_{h_{0}} + (m)_{-h_{0}}]^{2},$$
(18)

where $\xi_{\pm} = \sqrt{\Gamma^2 + (\pm h_0 + h^{\text{eff}})^2}$,

$$\kappa_{\pm} = \sqrt{\Gamma^2 + \left(\pm h_o + \frac{z}{z-1}h^{\text{eff}}\right)^2}$$

and, $(m)_{h_0}$ and $(m)_{-h_0}$ mean that in Eq. (14) h_i is taken to be equal to h_0 and $-h_0$, respectively.

III. RESULTS

The second-order phase transition lines can be obtained from the zero point of the coefficient of the second-order term in Eq. (18), when the equation is expanded in terms of h^{eff} . As a result, the second-order phase transition line is given by the nonlinear equation

$$\eta \beta' = \left(\frac{\gamma}{z-1}\right)^{1/2},\tag{19}$$

where

$$\begin{split} \eta &= z^2 \bigg(10H^2 \sqrt{G^2 + H^2} + 8H^2 \sqrt{G^2 + H^2} \cosh[\beta' \sqrt{G^2 + H^2}] + 2H^2 \sqrt{G^2 + H^2} \cosh[2\beta' \sqrt{G^2 + H^2}] \\ &\quad + \frac{1}{\beta'} \{ 3G^2 \sinh[\beta' \sqrt{G^2 + H^2}] + 4G^2 \sinh[2\beta' \sqrt{G^2 + H^2}] + 3G^2 \sinh[3\beta' \sqrt{G^2 + H^2}] \} \bigg), \\ \gamma &= 4z^5 (G^2 + H^2) (\cosh[\frac{1}{2}\beta' \sqrt{G^2 + H^2}] + \cosh[\frac{3}{2}\beta' \sqrt{G^2 + H^2}])^2 \{ 10\beta' G^2 H^2 + 10\beta' H^4 + 8\beta' H^2 (G^2 + H^2) \cosh[\beta' \sqrt{G^2 + H^2}] \\ &\quad + 2\beta' H^2 (G^2 + H^2) \cosh[2\beta' \sqrt{G^2 + H^2}] + 3G^2 \sqrt{G^2 + H^2} \sinh[\beta' \sqrt{G^2 + H^2}] + 4G^2 \sqrt{G^2 + H^2} \sinh[2\beta' \sqrt{G^2 + H^2}] \\ &\quad + 3G^2 \sqrt{G^2 + H^2} \sinh[3\beta' \sqrt{G^2 + H^2}] \}, \end{split}$$

 $\beta' = \beta z$, $G = \Gamma/z$, and $H = h_0/z$ are the dimensionless parameters, and J = 1 for simplicity.

There are two sensible cases for which the above formalism should be applied. The first case corresponds to the quantum transverse Ising model, which could be obtained by setting $h_0=0$, the second-order phase transition line is obtained by equating *H* equal to zero in Eq. (19),

$$\eta_1 \beta' = \left(\frac{\gamma_1}{z-1}\right)^{1/2},\tag{20}$$

where

$$\eta_1 = z^2 \frac{1}{\beta'} \{ 3G^2 \sinh[\beta'G] + 4G^2 \sinh[2\beta'G] + 3G^2 \sinh[3\beta'G] \},$$

and

$$\gamma_1 = 4z^5 G^2 (\cosh[\frac{1}{2}\beta'G] + \cosh[\frac{3}{2}\beta'G])^2 \{3G^3 \sinh[\beta'G] + 4G^3 \sinh[2\beta'G] + 3G^3 \sinh[3\beta'G]\}.$$

The second case corresponds to the random-field Ising model, which is obtained by taking $\Gamma = 0$. The second-order phase transition line is obtained by setting *G* equal to zero in Eq. (19),

$$\eta_2 \beta' = \left(\frac{\gamma_2}{z-1}\right)^{1/2},\tag{21}$$

where

$$\eta_2 = z^2 (10H^3 + 8H^3 \cosh[\beta' H] + 2H^3 \cosh[2\beta' H])$$
 and

$$\gamma_2 = 4z^5 H^2 (\cosh\left[\frac{1}{2}\beta'H\right] + \cosh\left[\frac{3}{2}\beta'H\right])^2 \{10\beta'H^4$$

$$+8\beta'H^4\cosh[\beta'H]+2\beta'H^4\cosh[2\beta'H]\}.$$

The second-order phase transition temperatures T are found iteratively from Eq. (19) by varying the random field H for given values of the transverse field G and the coordination number z. Similarly, the second-order phase transition temperatures T can also be obtained for the quantum transverse Ising model and the random-field Ising model by using Eqs. (20) and (21), respectively.

Besides the second-order phase transition lines, one should also investigate the possibility of the existence of tricritical points. In general, when the bimodal random field and transverse field are both present, the condition for the existence of tricritical points can be determined in the limiting case of $T=1/\beta' \rightarrow 0$ in the following manner: We expand the free energy, i.e., Eq. (18), in terms of the effective field h^{eff} , and then set the coefficients of the second-and fourthorder terms in the expansion to zero separately. As a result, two coupled equations are obtained and have to be solved numerically. Finally we obtain

$$G = \frac{3}{2} \frac{8}{5\sqrt{5}} \frac{z-1}{z},$$
 (22)

$$H = \frac{3}{2} \frac{4}{5\sqrt{5}} \frac{z-1}{z}.$$
 (23)

This results show that a tricritical point exists for $G < [\frac{3}{2}(8/5\sqrt{5})](z-1)/z$, and tricritical point disappears for $G > [\frac{3}{2}(8/5\sqrt{5})](z-1)/z$.

The phase diagrams of the bimodal random field quantum spin- $\frac{3}{2}$ Ising model for z = 4, 6, 8, 12, and ∞ (the MFA result)

are obtained using the above formalism for different values of the transverse field *G*, i.e., 0.0, 0.75, 0.85, 0.92, 0.96, 1.0, and 1.05 are given in Figs. 1(a)-1(g). As can be seen from the figure, the second-order phase transition temperature *T*, indicated by solid lines, is lowered on increasing the strength of the random field *H* until it reaches T=0 or ends at the tricritical points. The tricritical points are labeled with solid circles in the figure. It should also be notes that as *G* becomes larger the tricritical points appear at a lower *H*; eventually, according to the coordination number *z*, the tricritical points disappear.

When one decreases the random field, two successive phase transitions are observed; reentrant phenomena can be seen for appropriate values of G, and may be caused by quantum effects and randomness. The second-order phase transition temperature T, indicated by dotted lines, is lowered on decreasing the random field H from a higher value. These dotted lines terminate at a point in the region of the disordered phase indicated by solid rectangles, shown in the insets of the figures. This point which can be called an end point, appears at lower temperatures. When the random field is lowered from above, quantum effects mainly contribute and the transition from a disordered phase to an ordered phase is more characteristic of quantum spin transitions than the following one. When the random field decreases further, it becomes dominant, and a reentrance transition to the disordered phase may take place.

The behavior of the second-order phase transition lines for a spin- $\frac{3}{2}$ system is similar to the for spin- $\frac{1}{2}$ (Ref. 4) and spin-1 systems,¹² except near the zero second-order phasetransition temperatures. Both these models present reentrant behaviors as in the spin- $\frac{3}{2}$ case, but in the figures the end points of the dotted lines are not indicated. It should also be mentioned that Yokoto and Sugiyama,⁹ using the MFA, and Sarmento and Kaneyoshi,⁹ using an effective-field theory with correlation, studied the random-field transverse Ising model and obtained the tricritical point and reentrant behavior. It is also very interesting that the critical values of *G* and *H*, i.e., Eqs. (22), and (23), for the existence of the tricritical points are exactly $\frac{3}{2}$ times of the Eqs. (25) and (26) of the first of Refs. 11.

As a final note, it should be mentioned that the pair approximation is equivalent to the Bethe approximation, therefore, its free energy is lower than the MFA free energy. The pair approximation gives lower critical temperatures, but overestimates the tendency toward ordering as in the MFA. Figure 1 illustrates the changes of the phase diagrams for different values of z. When the coordination number z increases, it can be compared with the MFA results. In the limit $z \rightarrow \infty$, the ordinary MFA result for the quantum system is recovered. This may be caused by the pair approximation, taking into account the local structure of the interaction pattern of the system and its relation to the coordination number z of the lattice. However the MFA neglects the local structure of the pattern of interactions, and its calculations are valid only at high dimensions. This is the reason for the failure of the MFA (different pattern of the interactions can give the same thermodynamics²⁰). Finally, we should mention that

12

0.4

0.5

0.5

0.3

Н

12

0.3

н

12

0.3

н

0.4

0.4

0.5

(e)

0.6

(f)

0.6

(g)

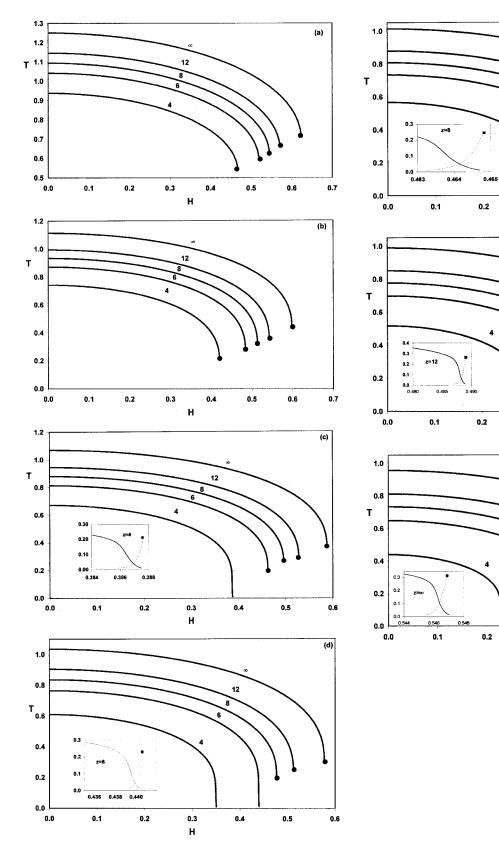


FIG. 1. In (a)–(g), the second-order phase transition lines, obtained in the (H, T) plane for the transverse fields G, are 0.0, 0.75, 0.85, 0.92, 0.96, 1.0, and 1.05, respectively. The lines are labeled with the values of the coordination number z. The solid and dotted lines correspond to the second-order phase transition lines with an increase and decrease of the random field H, respectively. The tricritical points are labeled with solid circles in the figures, and the end points of the dotted lines are indicated by solid rectangles in the insets.

the improved MFA (Ref. 21) for spin- $\frac{1}{2}$ systems includes the local structure for the TIM, but the results are too complicated with the random fields.

In conclusion, the bimodal random-field quantum spin- $\frac{3}{2}$ Ising system was studied extensively by combining the pair approximation with the DPIR. An analytical expression for the second-order phase transition temperature was obtained for the bimodal random field. Phase diagrams in the (*H*, *T*) plane were obtained numerically for some values of the transverse field *G* and the coordination number *z* by varying the random field *H*. It is shown that a tricritical point

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appears for $G < [\frac{3}{2}(\frac{8}{5}\sqrt{5})](z-1)/z$, and disappears for $G > [\frac{3}{2}(\frac{8}{5}\sqrt{5})](z-1)/z$. Reentrant phase transitions occur for appropriate ranges of *H* and *G*. By using the present formalism, one can also discuss the spin- $\frac{3}{2}$ Ising system with a trimodal random-field distribution.

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