Reentrant phase transitions in a quantum spin system with random fields

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The transverse Ising model with random fields has been studied within the mean-field approximation extended to include quantum effects. When applied random fields are bimodal (sum of two δ functions) and transverse fields Γ are not too large, tricritical points exist. In these cases, reentrant phenomena can be seen for appropriate ranges of Γ and random fields h_0.

I. INTRODUCTION

The random-field Ising model has been investigated, especially, regarding the problem of the lower critical dimension.[1] One of the other problems is how the form of random fields affects the structure of phase diagrams. From the latter point of view, the random-field Ising models with different types of random fields have been studied within the mean-field approximation. The transition for the Gaussian random field distribution is second order.[2] A tricritical point exists for the bimodal distribution.[3] A more complex phase diagram appears when random fields are trimodal (sum of three δ functions).[4] On the other hand, a quantum spin system with random fields at $T=0$ has been studied by the ϵ expansion.[5] The quantum-classical crossover is suppressed by the existence of random fields. As in classical systems, it is expected that the transition properties are affected by the shapes of random fields.

In this paper, the transverse Ising models with Gaussian and bimodal random fields are investigated by the combined use of the replica method for random systems and the extended mean-field method for quantum systems.[6] Full phase diagrams are obtained. In the Gaussian case, all of transitions are second order. On the other hand, in the bimodal case, tricritical points exist when transverse fields Γ are not too large. For larger values of Γ, transitions become second order. When random fields are bimodal types, reentrant phenomena occur if Γ and random fields h_0 are within appropriate ranges. This may be attributed to the competition between quantum effects and the randomness. When the temperature is lowered from above, quantum effects dominate and the transition from the disordered phase to the ordered phase is more characteristic of quantum spin transitions than the following one. And when the temperature is lowered further, the randomness dominates relatively, and the reentrant transition to the disordered phase could take place.

II. MODEL AND METHOD

A quantum spin system considered here is described by the following Hamiltonian:

$$\mathcal{H}=-J\sum_{\langle i,j\rangle}\sigma_i^z\sigma_j^z-\Gamma\sum_i\sigma_i^x-\sum_i h_i\sigma_i^z\ . \tag{1}$$

The summation in the first term is taken over nearest neighbor pairs. Γ is a transverse field, which represents quantum effects, and h_i is a random external field. The quenched partition function of this system can be rewritten as the corresponding partition function for the $(d+1)$-dimensional classical spin system by using the Suzuki-Trotter formula.[7] Here d is the original dimension of the quantum system. Then the partition function becomes

$$Z=\lim_{M\to\infty}\sum_{\{S_{i,m}=\pm1\}}\left[\frac{1}{2}\sinh\left[\frac{2\beta\Gamma}{M}\right]\right]^{MN/2}\times\exp\left\{\frac{\beta J}{M}\sum_{m=1}^{M}\sum_{\langle i,j\rangle}S_{i,m}S_{j,m}+\tfrac{1}{2}\ln\left[\coth\left[\frac{\beta\Gamma}{M}\right]\right]\sum_{m=1}^{M}\sum_i S_{i,m}S_{i,m+1}+\sum_{m=1}^{M}\sum_i\frac{\beta h_i}{M}S_{i,m}\right\}, \tag{2}$$

where m is the index for the Trotter direction and N is the total number of spins. Free energy can be calculated by the replica method as follows. The replicated partition function is given by

$$Z^n=\lim_{M_\alpha\to\infty}\sum_{\{S^\alpha_{i,m_\alpha}=\pm1\}}\prod_\alpha\left[\frac{1}{2}\sinh\left[\frac{2\beta\Gamma}{M_\alpha}\right]\right]^{M_\alpha N/2}$$

$$\times\exp\left\{\beta J\sum_\alpha\sum_{m_\alpha}\sum_{\langle i,j\rangle}\frac{1}{M_\alpha}S^\alpha_{i,m_\alpha}S^\alpha_{j,m_\alpha}+\sum_\alpha\tfrac{1}{2}\ln\left[\coth\left[\frac{\beta\Gamma}{M_\alpha}\right]\right]\sum_{m_\alpha}\sum_i S^\alpha_{i,m_\alpha}S^\alpha_{i,m_\alpha+1}\right.$$

$$\left.+\sum_\alpha\sum_{m_\alpha}\sum_i\frac{\beta h_i}{M_\alpha}S^\alpha_{i,m_\alpha}\right\}, \tag{3}$$

where α is the replica index. This quantity is averaged over random field distributions.

$$\langle Z^n\rangle_h=\int\{dh_i\}\prod_i p(h_i)Z^n\ , \tag{4}$$

where $p(h_i)$ represents distributions of random fields. Gaussian distributions are expressed by

$$p(h_i)=\frac{1}{\sqrt{2\pi}\sigma}e^{-h_i^2/2\sigma^2}\ . \tag{5}$$

Bimodal distributions can be represented by

$$p(h_i)=\tfrac{1}{2}[\delta(h_i-h_0)+\delta(h_i+h_0)]\ . \tag{6}$$

Although following explicit calculations will be performed for Gaussian distributions, the extension to other distributions is straightforward. In this case, (4) becomes

$$\langle Z^n\rangle_h=\lim_{M\to\infty}\sum_{\{S^\alpha_{i,m}=\pm1\}}\left[\frac{1}{2}\sinh\left[\frac{2\beta\Gamma}{M}\right]\right]^{nMN/2}$$

$$\times\exp\left\{\frac{\beta J}{M}\sum_\alpha\sum_m\sum_{\langle i,j\rangle}S^\alpha_{i,m}S^\alpha_{j,m}+\tfrac{1}{2}\ln\left[\coth\left[\frac{\beta\Gamma}{M}\right]\right]\sum_\alpha\sum_m\sum_i S^\alpha_{i,m}S^\alpha_{i,m+1}\right.$$

$$\left.+\frac{\sigma^2\beta^2}{2M}\sum_i(\sum_\alpha\sum_m S^\alpha_{i,m})^2\right\}. \tag{7}$$

The mean-field approximation extended for quantum systems[6] is applied to this model. The key point in the extended mean-field method is to take account of the finiteness in the Trotter direction by solving the one-dimensional problem along the direction, and hence quantum effects are included satisfactorily in mean-field approximations. Generally, mean-field approximations correspond to take saddle points in the steepest-descent method. The following identity is used to apply the steepest-descent method:

$$1=\int_{-\infty}^{\infty}d\Phi^\alpha_{i,m}\delta(S^\alpha_{i,m}-\Phi^\alpha_{i,m})=\frac{1}{2\pi i}\int_{-\infty}^{\infty}d\Phi^\alpha_{i,m}\int_{-i\infty}^{i\infty}dK^\alpha_{i,m}\exp[(S^\alpha_{i,m}-\Phi^\alpha_{i,m})K^\alpha_{i,m}]\ . \tag{8}$$

Using this identity, (7) is rewritten as follows:

$$\langle Z^n\rangle_h=\lim_{M\to\infty}\left[\frac{1}{2}\sinh\left[\frac{2\beta\Gamma}{M}\right]\right]^{nMN/2}\int\prod_i\prod_m\prod_\alpha\frac{1}{2\pi i}d\Phi^\alpha_{i,m}dK^\alpha_{i,m}\exp\left[\frac{\beta J}{M}\sum_\alpha\sum_m\sum_{\langle i,j\rangle}\Phi^\alpha_{i,j}\Phi^\alpha_{j,m}\right.$$

$$\left.-\sum_\alpha\sum_m\sum_i K^\alpha_{i,m}\Phi^\alpha_{i,m}+\sum_i W_0(K^\alpha_{i,m})\right]. \tag{9}$$

Here $W_0(K^\alpha_{i,m})$ is defined by

$$e^{W_0(K^\alpha_{i,m})}\equiv\sum_{\{S^\alpha_{i,m}=\pm1\}}\exp\left\{\sum_\alpha\sum_m K^\alpha_{i,m}S^\alpha_{i,m}+\tfrac{1}{2}\ln\left[\coth\left[\frac{\beta\Gamma}{M}\right]\right]\sum_\alpha\sum_m S^\alpha_{i,m}S^\alpha_{i,m+1}+\frac{\sigma^2\beta^2}{2M}\left[\sum_\alpha\sum_m S^\alpha_{i,m}\right]^2\right\}. \tag{10}$$

Then saddle-point conditions become

$$\left.\frac{\partial W_0(K^{\alpha}_{i,m})}{\partial K^{\alpha}_{i,m}}\right|_{(K^{\alpha}_{i,m})^*}=(\Phi^{\alpha}_{i,m})^*,\quad \frac{\beta J}{M}\sum_{\substack{j\\ \langle i,j\rangle}}\Phi(^{\alpha}_{j,m})^*=K(^{\alpha}_{i,m})^* , \tag{11}$$

where the asterisk represents the value at a saddle point. If saddle points are assumed to be independent of i, α, and m, (11) becomes

$$\left.\frac{\partial W_0(K^{\alpha}_{i,m})}{\partial K^{\alpha}_{i,m}}\right|_{K^{\alpha}_{i,m}=K^*}=\Phi^*,\quad \frac{2d\beta J}{M}\Phi^*=K^* . \tag{12}$$

At saddle points, (10) becomes

$$e^{W_0(K^*)}=\sum_{\{S^{\alpha}_{i,m}=\pm 1\}}\exp\left\{\frac{1}{2}\ln\left[\coth\left[\frac{\beta T}{M}\right]\right]\sum_{\alpha}\sum_{m}S^{\alpha}_{m}S^{\alpha}_{m+1}+K^*\sum_{\alpha}\sum_{m}S^{\alpha}_{m}\right\}$$
$$\times\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}ds\,\exp\left[-\frac{1}{2}s^2+\frac{\sigma\beta}{M}\left[\sum_{\alpha}\sum_{m}S^{\alpha}_{m}\right]s\right]$$
$$=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}ds\,e^{-s^2/2}\left[\sum_{\{S_m=\pm 1\}}\exp\left\{\frac{1}{2}\ln\left[\coth\left[\frac{\beta\Gamma}{M}\right]\right]\sum_{m}S_mS_{m+1}+\left[K^*+\frac{\sigma\beta s}{M}\right]\sum_{m}S_m\right\}\right]^n . \tag{13}$$

Here inside the brace is the partition function for the Ising chain in external fields with the periodic boundary condition. This can be solved by the transfer-matrix method.[8] Using the eigenvalues of the transfer-matrix λ_+ and λ_-, (13) can be rewritten as

$$e^{W_0(K^*)}=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}ds\,e^{-s^2/2}(\lambda_+^M+\lambda_-^M)^n . \tag{14}$$

Here $\lambda_\pm$ are expressed by

$$\lambda\pm=\left[\coth\left[\frac{\beta\Gamma}{M}\right]\right]^{1/2}\cosh\left[K^*+\frac{\sigma\beta s}{M}\right]\pm\left[\coth\left[\frac{\beta\Gamma}{M}\right]\sinh^2\left[K^*+\frac{\sigma\beta s}{M}\right]+\tanh\left[\frac{\beta\Gamma}{M}\right]\right]^{1/2} . \tag{15}$$

Hereafter, the mean-field approximation for $\langle Z^n\rangle_h$ is expressed by $\langle Z_0^n\rangle_h$. Using the second equation of (12), $\langle Z_0^n\rangle_h$ is given by

$$\langle Z_0^n\rangle_h=\lim_{M\to\infty}\left[\frac{1}{2}\sinh\left[\frac{2\beta\Gamma}{M}\right]\right]^{nMN/2}\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}ds\,e^{-s^2/2}(e^{-d\beta J\Phi^{*2}})^n\times(\lambda_+^M+\lambda_-^M)^n\right]^N . \tag{16}$$

The mean-field approximation for the free energy per spin F_0 becomes

$$F_0=-\frac{\langle\ln Z_0\rangle_h}{\beta N}=-\frac{1}{\beta N}\lim_{n\to 0}\frac{\langle Z_0^n\rangle_h-1}{n}$$
$$=dJ\Phi^{*2}-\frac{1}{\beta}\lim_{M\to\infty}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}ds\,e^{-s^2/2}\left\{\ln\left[\frac{1}{2}\sinh\left[\frac{2\beta\Gamma}{M}\right]\right]^{M/2}+\ln(\lambda_+^M+\lambda_-^M)\right\}$$
$$=dJ\Phi^{*2}-\frac{1}{\beta}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}ds\,e^{-s^2/2}\ln(2\cosh\{\beta[(2dJ\Phi^*+\sigma s)^2+\Gamma^2]^{1/2}\}) . \tag{17}$$

The averaged magnetization is obtained by solving the equation

$$\Phi^*=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}ds\,e^{-s^2/2}\frac{(2dJ\Phi^*+\sigma s)}{[(2dJ\Phi^*+\sigma s)^2+\Gamma^2]^{1/2}}\tanh\{\beta[(2dJ\Phi^*+\sigma s)^2+\Gamma^2]^{1/2}\} . \tag{18}$$

Among solutions, the real magnetization minimizes the free energy (17). In the case of bimodal random field distributions, similar equations can be obtained, so (17) and (18) are generally written as

$$F_0=dJ\Phi^{*2}-\frac{1}{\beta}\int dh\,p(h)\ln(2\cosh\{\beta[(2dJ\Phi^*+h)^2+\Gamma^2]^{1/2}\}) , \tag{19}$$

$$\Phi^*=\int dh\,p(h)\frac{(2dJ\Phi^*+h)}{[(2dJ\Phi^*+h)^2+\Gamma^2]^{1/2}}\tanh\{\beta[(2dJ\Phi^*+h)^2+\Gamma^2]^{1/2}\} . \tag{20}$$

To investigate the bimodal case for some extreme values of parameters, the right-hand side of (20) is defined as $f(\Phi^*)$. The possibility of the existence of tricritical points can be examined by expanding $f(\Phi^*)$ in Φ^*. The first derivative of $f(\Phi^*)$ at the origin is given by

$$f'(0)=\frac{G^2}{(H^2+G^2)^{3/2}}\tanh\frac{(H^2+G^2)^{1/2}}{T}+\frac{H^2}{T(H^2+G^2)}\operatorname{sech}^2\frac{(H^2+G^2)^{1/2}}{T}\ , \tag{21}$$

where the dimensionless parameters

$$T\equiv\frac{1}{\beta\times 2dJ},\quad G\equiv\frac{\Gamma}{2dJ},\quad H\equiv\frac{h_0}{2dJ} \tag{22}$$

are used. If transitions are second order, $f'(0)=1$ represents transitions. Possible tricritical points can be read from the following third derivative of $f(\Phi^*)$ at the origin:

$$\begin{aligned}f^{(3)}(0)=&\frac{3G^2(4H^2-G^2)}{(H^2+G^2)^{7/2}}\tanh\frac{(H^2+G^2)^{1/2}}{T}+\frac{3G^2(G^2-4H^2)}{T(H^2+G^2)^3}\operatorname{sech}^2\frac{(H^2+G^2)^{1/2}}{T}\\&-\frac{12G^2H^2}{T(H^2+G^2)^{5/2}}\operatorname{sech}^2\frac{(H^2+G^2)^{1/2}}{T}\tanh\frac{(H^2+G^2)^{1/2}}{T}\\&+\frac{4H^4}{T^2(H^2+G^2)^2}\operatorname{sech}^2\frac{(H^2+G^2)^{1/2}}{T}-\frac{6H^4}{T^2(H^2+G^2)^2}\sec^4\frac{(H^2+G^2)^{1/2}}{T}\ .\end{aligned} \tag{23}$$

Candidates for tricritical points correspond $f^{(3)}(0)=0$ with $f'(0)=1$. Next, three cases are examined explicitly.

In the case of $T=0$, $f'(0)$ and $f^{(3)}(0)$ are given by

$$f'(0)=\frac{G^2}{(H^2+G^2)^{3/2}}\ , \tag{24}$$

$$f^{(3)}(0)=\frac{3G^2(4H^2-G^2)}{(H^2+G^2)^{7/2}}\ . \tag{25}$$

So the following point could be a tricritical point:

$$G=(\tfrac{4}{5})^{3/2},\quad H=\frac{4}{5\sqrt{5}}\ . \tag{26}$$

The second case is $G=0$. From (21) and (23), $f'(0)$ and $f^{(3)}(0)$ are given by

$$f'(0)=\frac{1}{T}\operatorname{sech}^2\left[\frac{H}{T}\right]\ , \tag{27}$$

$$f^{(3)}(0)=\frac{2}{T^2}\operatorname{sech}^2\left[\frac{H}{T}\right]\left[3\tanh^2\left[\frac{H}{T}\right]-1\right]\ . \tag{28}$$

By using these quantities, a tricritical point could appear at the following point, which is same as the one obtained by Aharony:[3]

$$T=\tfrac{2}{3},\quad H=\tfrac{2}{3}\operatorname{arctanh}\sqrt{1/3}\ . \tag{29}$$

$H=0$ is the last case, in which $f'(0)$ and $f^{(3)}(0)$ are given by

$$f'(0)=\frac{1}{G}\tanh\frac{G}{T}\ , \tag{30}$$

$$f^{(3)}(0)=-\frac{1}{G^3}\tanh\frac{G}{T}+\frac{3}{TG^2}\operatorname{sech}^2\left[\frac{G}{T}\right]\ . \tag{31}$$

On the second-order transition line, (31) can be written as

$$f^{(3)}(0)=\frac{3}{TG^2}\left[1-\frac{G}{\operatorname{arctanh}G}-G^2\right]\ . \tag{32}$$

This quantity can be proved to be negative for $0<G<1$. So, the transition is second order in this case.

III. RESULTS

Phase diagrams will be obtained by solving (20) numerically. Among the solutions, the real magnetization minimizes the free energy (19). Phase diagrams for two types of random field distributions are obtained.

A. Gaussian distributions

In Fig. 1, the phase diagram for Gaussian random field distributions is given. Here the same notation as the bi-

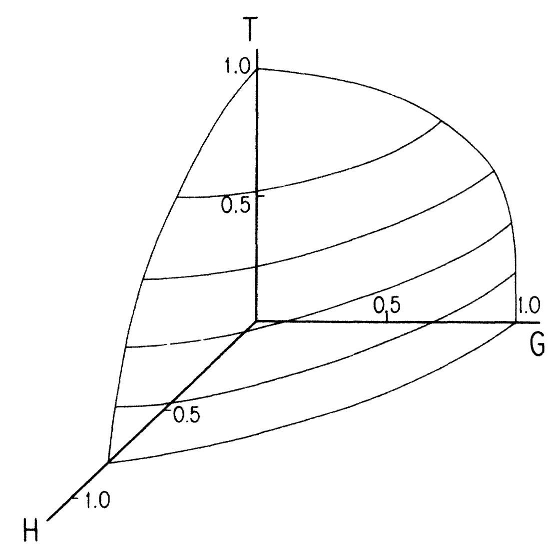

FIG. 1. The phase diagram for Gaussian random field distributions. Dimensionless parameters defined in Eqs. (22) are used except for H. Here H is defined by $\sigma/2dJ$. The ferromagnetic phase includes the origin. All the transitions are second order.

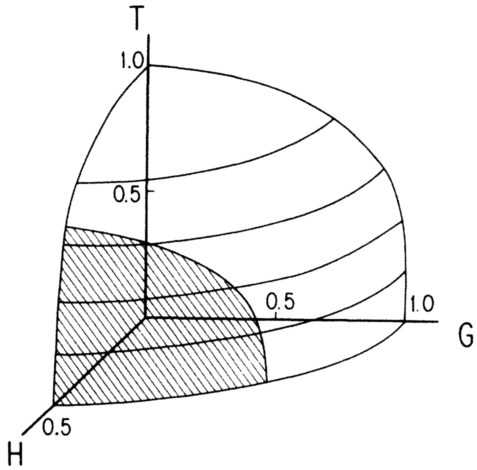

FIG. 2. The phase diagram for bimodal random field distributions. Dimensionless parameters defined in Eqs. (22) are used. The ferromagnetic phase includes the origin. First-order transitions occur at the shaded surface. At other parts of the surface, transitions are second order.

modal case is used for $H \equiv \sigma/2dJ$. The ferromagnetic phase includes the origin. All the transitions are second order.

B. Bimodal distributions

The phase diagram for bimodal distributions is shown in Fig. 2. The ferromagnetic phase includes the origin. First-order transitions occur at the shaded surface. At other parts of the surface, transitions are second order. Looking at the phase diagram in a H-T plane for a fixed G, a tricritical point exists for $G < (\frac{4}{5})^{3/2}$ from the results of (26). On the other hand, no tricritical points appear for $G > (\frac{4}{5})^{3/2}$. Reentrant phase transitions can be seen explicitly for appropriate values of G. Three examples are shown in Fig. 3. Figure 3(a), 3(b), and 3(c) correspond to $G = 0.6$, 0.678, and 0.72, respectively. Solid lines represent second-order transitions and broken lines represent first-order ones. When the temperature is lowered from above, disorder to order transitions occur at first. Reentrant phenomena can be seen by lowering the temperature further. The origin of reentrance is not so clear, but may be thought of as follows. Both quantum effects and the randomness prevent ordering, but the two effects do not affect in the same manner as is seen from (20). The transition in which the randomness dominates has the tendency to be first order. Quantum effects tend to make it second order. So, when the temperature is lowered from above, the randomness does not work relatively at first and the transition is more characteristic of the quantum spin transition than the succeeding one. And if the temperature is lowered further, the randomness contribute mainly and the reentrance to the disordered phase may take place. Further investigations are needed to clarify the mechanism of the reentrance transition including the reason why it cannot be seen in the Gaussian random field distributions.

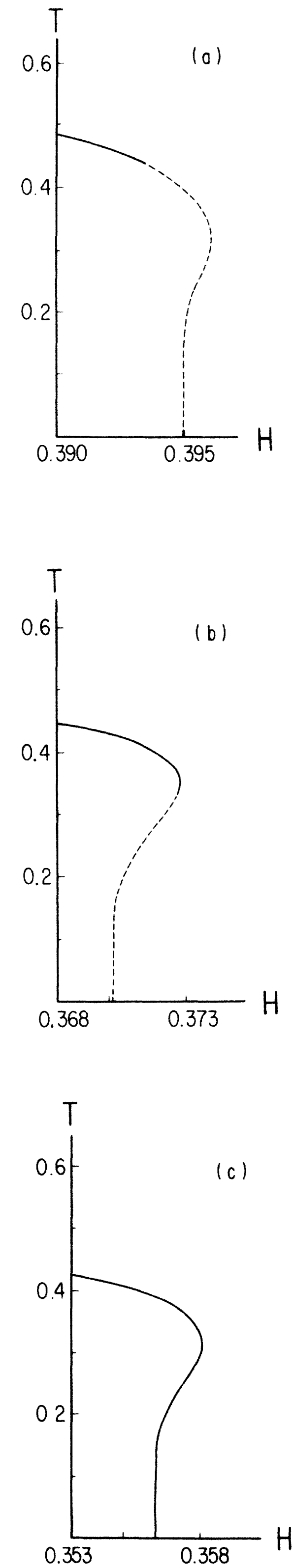

FIG. 3. Three examples which exhibit reentrant phase transitions. Dimensionless parameters defined in Eqs. (22) are used. (a), (b), and (c) correspond to $G = 0.6$, 0.678, and 0.72, respectively. Solid lines represent second-order transitions and broken lines represent first-order ones.

C. Summary

The mean-field method extended for quantum models has been applied to the random system successfully by using the Suzuki-Trotter formula and the replica method. Quantum effects are included by solving the one dimensional problem along the Trotter direction. In the case of Gaussian random field distributions, no tricritical points exist. On the other hand, a tricritical point appear for $G<(\frac{4}{5})^{3/2}$ in the bimodal case. In this case, reentrant phase transitions, which may be caused by the competition between quantum effects and the randomness, occur for appropriate ranges of h_0 and Γ.

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