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Longitudinal and transverse random-field Ising model

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Abstract. The Ising model with both random longitudinal and transverse fields is studied by combining the pair approximation with the discretized path integral representation. The phase diagrams of the spin $S = \frac{1}{2}$ system are obtained; the relations between the critical temperature and the local structure as well as the tricritical and re-entrant phenomena are discussed.

1. Introduction

Since de Gennes introduced the transverse Ising model to explain the phase transition of hydrogen-bonded ferroelectrics such as KH_2PO_4 in the order–disorder phenomenon with tunnelling effects [1], it has been successfully used to study a number of problems of phase transitions associated with order–disorder phenomena in other systems (a more detailed application has been reviewed in [2]). The model is described by the Ising Hamiltonian to which is added a term which represents the effects of the transverse field part. Owing to the requisite non-commutativity of operators in the Hamiltonian, deriving the eigenvalues of the Hamiltonian is very difficult. Therefore, many theorists have used various methods to investigate this problem [3–7], such as the mean-field approximation, the effective-field theory, the renormalization group method, Monte Carlo simulation, and the method of combining the pair approximation with the discretized path integral representation (DPIR). Many interesting phenomena have been investigated.

Recently, the transverse random-field Ising model (TRFIM) has received much attention. Cassol *et al* [8] have studied the phase diagram and found a finite discontinuity in the phase diagram at $T = 0$, between the trimodal and bimodal random distributions of the transverse field. Subsequently, Yokota [9] pointed out that the directional randomness of the transverse field does not change the critical behaviour.

A large number of papers have focused on the transverse Ising model with a random longitudinal field in the presence of a fixed transverse field, and its properties have been investigated in detail [6, 7]. However, the properties of the Ising model with both longitudinal and transverse random fields have not been reported. We know that the form of the random-longitudinal-field distribution plays an important role in the determination of the order of phase transition; on the other hand, the transverse field gives rise to a possible spin-flip transition and hence works against the ordering. What will happen when both the transverse and the longitudinal fields are randomly distributed? How does this change the phase diagram? This is our goal in the present work. For the case when the spin $S = \frac{1}{2}$, we

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use a method which combines the pair approximation with DPIR [10–12] to investigate the critical behaviour of the Ising model with longitudinal and transverse random fields which are bimodally and trimodally distributed, respectively.

2. Theory

For an Ising model with both longitudinal and transverse random fields, the total Hamiltonian of the system is given by

$$H = -J\sum_{i,j} S_i^z S_j^z - \sum_i \Gamma_i S_i^x - \sum_i h_i S_i^z \tag{1}$$

where S_i^x and S_i^z are the quantum spin (S) operators at site i, the summation in the first term is taken over every nearest-neighbour pair of spins only once, h_i is the longitudinal random field at site i with the symmetric bimodal distribution of the probability given by

$$P(h_i) = \tfrac{1}{2}[\delta(h_i - h) + \delta(h_i + h)] \tag{2a}$$

and Γ_i in equation (1) represents the transverse random field at site i with the trimodal distribution of the probability given by

$$P(\Gamma_i) = p\delta(\Gamma_i) + \frac{1-p}{2}[\delta(\Gamma_i - \Gamma) + \delta(\Gamma_i + \Gamma)] \tag{2b}$$

where the parameter p measures the fraction of spins in the system not exposed to the transverse field. Γ represents a uniform transverse magnetic field.

The effective Hamiltonian for a pair of nearest-neighbour spins i and j in the pair approximation can be written in the form [13]

$$H^{(2)} = -JS_i^z S_j^z - \Gamma_i S_i^x - (h_i + h_i^{\text{eff}})S_i^z - \Gamma_j S_j^x - (h_j + h_j^{\text{eff}})S_j^z \tag{3}$$

where h^{eff} is the local molecular field on site i coming from spins at all other sites except from site j. For simplicity, we suppose that h^{eff} is independent of the sites.

In order to obtain the pair partition function, we shall reformulate the Hamiltonian in the DPIR. The idea in the DPIR is to convert the quantized two-state spin on each lattice site into a P-component vector $\hat{\mathbb{U}}$ ($\mathbb{U}^{(1)}, \mathbb{U}^{(1)}, \ldots, \mathbb{U}^{(P)}$) and eventually to let P go to infinity. Each component $\mathbb{U}^{(t)}(t = 1, 2, \ldots, P)$ is taken to be a classical two-state variable $\mathbb{U}^{(t)} = \pm 1$, and the net effect is to represent the quantum uncertainty by creating many copies, or replicas, of the original variable [10–12]. By means of the DPIR, the pair Hamiltonian can be split into a reference part $H_0^{(2)}$ of a one-body Hamiltonian plus a two-body interaction part V.

The corresponding free energy can be expressed in terms of the free energy of the reference part and the cumulant expansion in the reference part:

$$-\beta F = \ln\{\text{Tr}[\exp(-\beta H^{(2)})]\} = -\beta F_0 + \sum_{n=1}^{\infty}(-\beta)^n C_n(V) \tag{4}$$

with $-\beta F_0 = \ln\{\text{Tr}[\exp(-\beta H_0^{(2)})]\}$ and the cumulants are given by $C_1(V) = \langle V\rangle_0$, $C_2(V) = \langle V^2\rangle_0 - \langle V\rangle_0^2, \ldots$, where $\langle\cdots\rangle_0$ indicates an average over the reference part.

The pair partition function may be evaluated from

$$\ln Q^{(2)} = \ln\{\mathrm{Tr}[\exp(-\beta H^{(2)})]\}$$

$$= \ln[[2\cosh\{\beta[(h_i + h^{\mathrm{eff}})^2 + \Gamma_i^2]^{1/2}\}]] + \ln[[2\cosh\{\beta[(h_j + h^{\mathrm{eff}})^2 + \Gamma_j^2]^{1/2}\}]]$$

$$+ \beta J \frac{\tanh\{\beta[(h_i + h^{\mathrm{eff}})^2 + \Gamma_i^2]^{1/2}\}}{[(h_i + h^{\mathrm{eff}})^2 + \Gamma_i^2]^{1/2}}(h_i + h^{\mathrm{eff}})$$

$$\times \frac{\tanh\{\beta[(h_j + h^{\mathrm{eff}})^2 + \Gamma_j^2]^{1/2}\}}{[(h_j + h^{\mathrm{eff}})^2 + \Gamma_j^2]^{1/2}}(h_j + h^{\mathrm{eff}}). \tag{5}$$

The effective Hamiltonian for the ith spin is of the form [13]

$$H^{(1)} = -\Gamma_i S_i^x - (h_i + H^{\mathrm{eff}})S_i^z \tag{6}$$

where H^{eff} is the one-body effective field at site i, and H^{eff} is related to h^{eff} as follows: $H^{\mathrm{eff}} = [Z/(Z-1)]h^{\mathrm{eff}}$ (Z is the coordination number).

The corresponding single-spin partition function is

$$Q^{(1)} = 2\cosh\{\beta[(h_i + H^{\mathrm{eff}})^2 + \Gamma_i^2]^{1/2}\}. \tag{7}$$

The free energy of the full system is given by the expression [14]

$$\frac{-\beta\langle F(h^{\mathrm{eff}})\rangle_{h,\Gamma}}{N} = \langle \ln Q^{(1)}\rangle_{h,\Gamma} + \frac{Z}{2}(\langle \ln Q^{(2)}\rangle_{h,\Gamma} - \langle \ln Q^{(1)}\rangle_{h,\Gamma}) \tag{8}$$

where $\langle\cdots\rangle_{h,\Gamma}$ is the average over distributions of longitudinal and transverse random fields. According to the Landau second-order phase transition theory, when the average free energy is expanded in terms of h^{eff} (as an order parameter), the second-order phase transition equation can be determined from when the expanding coefficient of the second-order term $(h^{\mathrm{eff}})^2$ vanishes in equation (8).

By introducing the dimensionless parameters

$$G \equiv \frac{\Gamma}{ZJ} \qquad H \equiv \frac{h}{ZJ} \qquad T \equiv \frac{1}{\beta ZJ} \tag{9}$$

the equation determining the second-order phase transition can be written as [10]

$$(1-p)\left[\frac{G^2}{(G^2+H^2)^{3/2}}\tanh\left(\frac{(G^2+H^2)^{1/2}}{T}\right) + \frac{H^2}{T(H^2+G^2)}\operatorname{sech}^2\left(\frac{(G^2+H^2)^{1/2}}{T}\right)\right]$$

$$+ \frac{p}{T}\operatorname{sech}^2\left(\frac{H}{T}\right) = \frac{Z}{Z-1}. \tag{10}$$

3. Results and discussion

The conditions for the existence of tricritical points can be obtained in the limit case of $T \to 0$ [15, 16]. We expand the free energy (equation (8)) up to the fourth-order term of h^{eff} and then set the coefficient of the second- and fourth-order terms in the expansion to zero separately. The existence of a tricritical point will be determined unambiguously from the two coupled equations

$$\frac{4p}{G_0^5} = \frac{G_0^2 - H_0^2}{(G_0^2 + H_0^2)^{7/2}} \tag{11}$$

and

$$\frac{(1-p)G_0^2}{(G_0^2 - H_0^2)^{3/2}} = \frac{Z}{Z-1}. \tag{12}$$

From these equations, the critical values of G_0 and H_0 of the transverse and longitudinal fields may be determined. We find that a critical point may exist only when $0 \leqslant p < 0.2$ and $G < G_0$ with $H > H_0$. The change in the critical values of G_0 and H_0 with p is shown in figure 1.

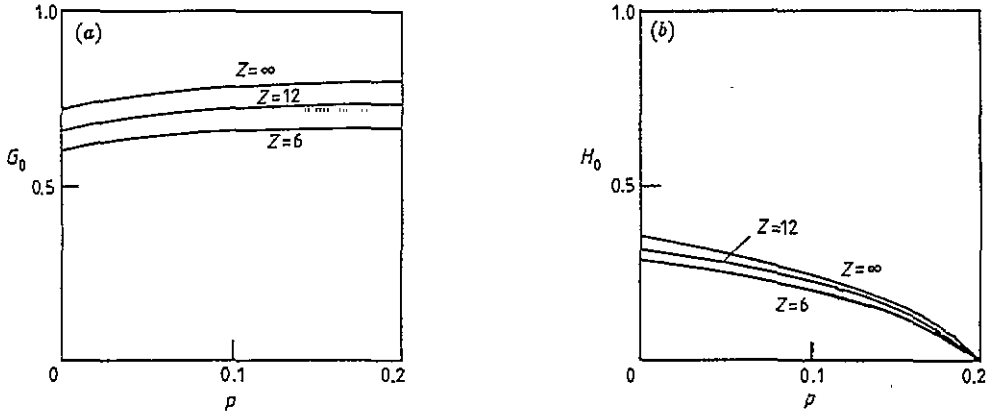

Figure 1. The changes in the critical values G_0 and H_0 with p for $Z = 6$, 12 and ∞.

The phase diagrams of the change in phase transition temperature with the transverse field for the case with the longitudinal field are shown in figures 2 and 3.

First, we consider the case $H = 0$ which is similar to that in [8]. For the case $Z = 6$, the phase diagram is shown in figure 2, which is in agreement with that in [8]. For $p = 0$ i.e. the transverse random field is a bimodal distribution, the critical transverse field Γ_c for which $T_c = 0$ does exist. We obtain that the values of the critical transverse field Γ_c and critical transition temperature T_c (when $\Gamma = 0$) are $\Gamma_c = 5.04J$ and $T_c = 4.92J$. The results are comparable with series expansion results [15]: $\Gamma_c = 5.16J$ and $T_c = 4.54J$. It can be seen that our results are better than the results obtained in [8]: $\Gamma_c = 5.33J$; $T_c = 4.93J$. The reason is that the lattice–spin interaction has been taken into account in our method of calculation.

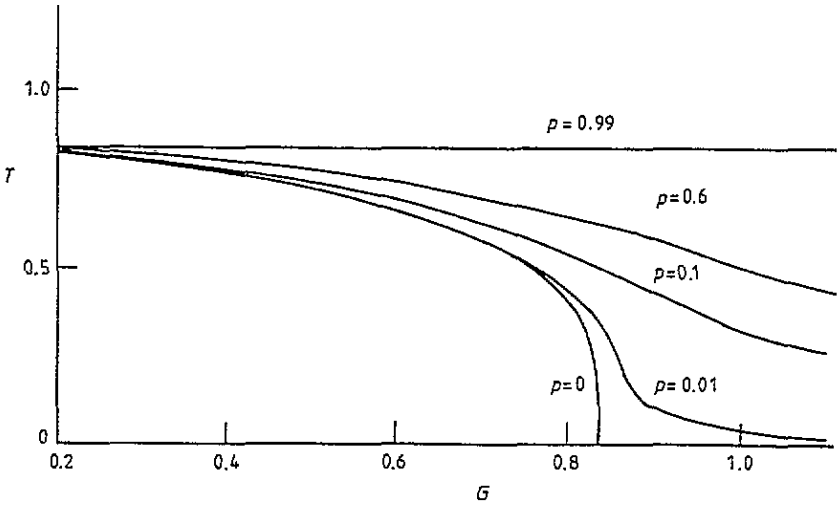

Figure 2. Phase diagram in the (T, G) plane for $Z = 6$, $H = 0$ and $p = 0$, 0.01, 0.1, 0.2, 0.6 and 0.99.

When the transverse random field is taken as a trimodal distribution (i.e. $p \neq 0$), there is no critical transverse field. This indicates that the thermodynamic properties of the system are discontinuous between the two different cases, $p = 0$ and $p \neq 0$. The pair approximation takes into account the local structure of the interaction on the pattern of the underlying system, which results in coordination-dependent phase diagrams. We believe that a discontinuity between the bimodal and trimodal distributions of the transverse field at $T = 0$ exists in the TRFIM.

Secondly, when the form of the random longitudinal field is taken to be a bimodal distribution, the discontinuity mentioned above will disappear. The phase diagram shown in figure 3 is different from that in the absence of the longitudinal field H. When H is very small (e.g. $H < 0.05$), the result obtained is similar to the case $H = 0$. If the longitudinal field increases to a large value (such as $H = 0.2$), the phase diagrams in figure 3 show that, for the case $p = 0$, the critical transverse field exists; however, there is no re-entrant phenomenon and no tricritical point. For $0 < p \ll 1$, the re-entrant phenomenon and re-entrant tricritical point may occur and become more spectacular when p increases to a certain value. For larger p, there is no critical transverse field. On the other hand, the value of the critical transverse field increases as the coordination number Z increases. The phase diagrams in figure 3 display the relation between the transition temperature and the local structure. If the longitudinal field is sufficiently large, we shall find that, even when $p = 0$, the re-entrant phenomenon and re-entrant tricritical point may also occur.

Furthermore, the phase diagrams for $Z = 6$, 12 and ∞ in the (T, H) plane are shown in figures 4(*a*), 4(*b*) and 4(*c*), corresponding to $G = 0.6$, 0.678 and 0.72, respectively, where the influence of the random distributed transverse field on the critical behaviour of the system is investigated. Our model may also be seen as a random-longitudinal-field Ising model (RLFIM) with a trimodal random distribution of the transverse field, which is different from the RLFIM model with a fixed transverse field. We shall now compare the results with those in [10], where a bimodal random-longitudinal-field Ising model with a fixed transverse field is studied. For trimodally distributed transverse fields in which the value of the reduced uniform transverse field is taken to be the same as the value of the

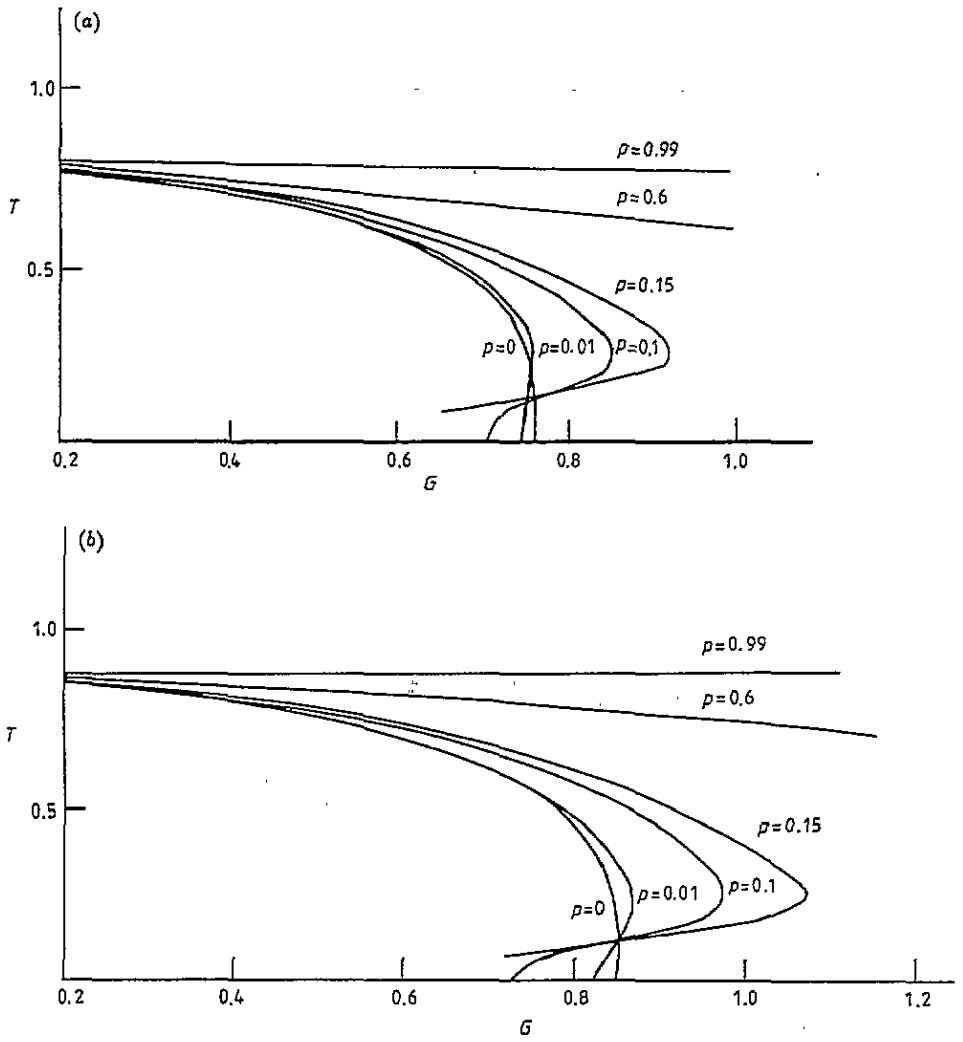

Figure 3. Phase diagram in the (T, G) plane for $H = 0.2$, $p = 0$, 0.01, 0.1, 0.15, 0.6 and 0.99: (*a*) $Z = 6$; (*b*) $Z = 12$.

fixed reduced transverse field in [10], we find that the critical values of random transverse fields at which tricritical points may exist are larger than those of the RLFIM in the presence of a fixed transverse field. Relatively speaking, the tricritical points are easy to observe. On the other hand, critical values of the random transverse field where the phase transition temperature $T_c = 0$ is lower, e.g. in figure 4(*b*), for $Z = 6$, $G_c = 0.222$ is less than $G_c = 0.26$ for a fixed transverse field, and the re-entrant phenomenon is more spectacular.

As we know, the re-entrant transition may be attributed to competition between the quantum fluctuation and randomness; the quantum fluctuation is induced by the transverse field and the randomness is caused by the random distributions of transverse and longitudinal fields. However, the two effects do not operate in the same manner when the temperature decreases. When the temperature is reduced, quantum fluctuations dominate and the transition from the disordered phase to the ordered phase is more characteristic of a quantum

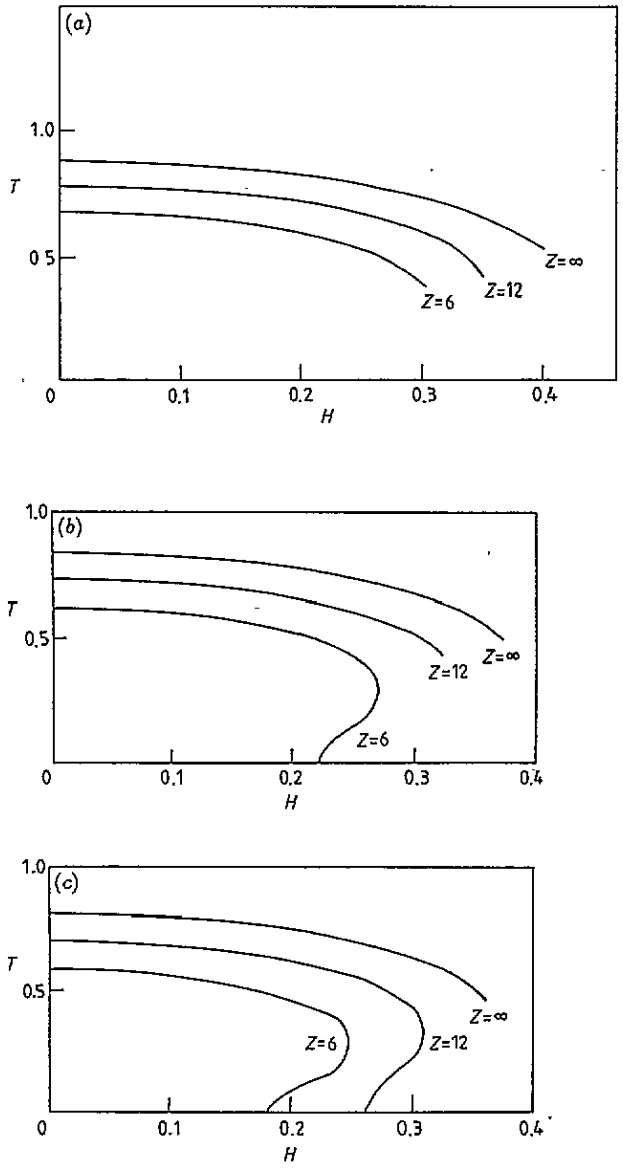

Figure 4. Phase diagram in the (T, H) plane for $p = 0.05$ and $Z = 6$, 12 and ∞: (a) $G = 0.6$; (b) $G = 0.678$; (c) $G = 0.72$.

spin transition. If the temperature is decreased further, the random fields dominate and a re-entrant transition to the disordered phase may take place. As p increases, the probability of disappearance of the transverse field at some sites is increased and the quantum effect is relatively weaker, but the randomness of the transverse random field distribution increases (to a certain extent); therefore, the re-entrant phenomenon may take place even when the transverse field is large, i.e. the re-entrant phenomennon is more spectacular. If p increases further, the quantum effects will be very weak, and at the same time the randomness is reduced; therefore, if the transverse field magnitude increases, the re-entrant phenomenon will disappear.

For the RLFIM with a random transverse field, the tricritical and re-entrant phenomena may occur. However, there are some differences in the phase diagram between the RLFIM with a random transverse field and with a fixed transverse field.

So far, we have calculated the phase diagrams for the Ising model with both longitudinal and transverse random fields. We have selected the bimodal distribution of probability for the random longitudinal field. The form of the random-field distribution has an important effect on the phase diagrams of the system.

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