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Transverse freezing in the infinite-range quantum Ising spin glass with transverse and Gaussian random longitudinal fields

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Abstract. The infinite-range quantum Ising spin glass in a transverse and a Gaussian random field has been studied by combining the pair approximation with the discretized path-integral representation. The phase diagrams are obtained, and the possibilities of the existence of a mixed phase in which ferromagnetism and spin-glass order coexist are discussed. This is expected to interpret some properties of the mixed hydrogen-bonded ferroelectric and antiferroelectric crystals such as $Rb_{1-x}(NH_4)_xH_2PO_4$.

Recently there has been much interest in the quantum version of the Sherrington–Kirkpatrick Ising spin glass (SG) in a transverse field [1–15]. This model is expected to describe some SG properties in non-magnetic cases, such as the mixed hydrogen-bonded ferroelectrics and antiferroelectrics of the $Rb_{1-x}(NH_4)_xH_2PO_4$ (RADP type—the so-called proton glasses [4, 13]. Here the proton tunnels between the two energy minima in the hydrogen bond, which is mimicked by the transverse field. Some workers have obtained the transverse freezing temperature for the symmetric transverse Ising SG (i.e. the model corresponding to $x = \frac{1}{2}$ in RADP). The paramagnetic and SG phases are separated by a line of instability [1, 7], which is analogous to the Gabay–Toulouse line), characterized by a freezing of the spin components which are transverse with respect to the applied field [16]. However, since a transverse field Γ applied in the Ising spin system brings about a quantum effect by causing spin flips, the requisite non-commutativity of operators in the Hamiltonian creates a potentially difficult technical problem [17]. It turns out that the statics and dynamics within the replica theory cannot give a complete phase diagram in fully deuterated RADP, which can be conveniently described by a quantum transverse Ising model with quenched random infinite-range interactions and intrinsic quenched random fields generated by substitutional impurities. In a previous paper [18], we have proposed a new approach, which combines the pair approximation for random Ising system and the discretized path-integral representation (DPIR) for quantum spin systems, to study the effect of a transverse field Γ on the paramagnetic-to-SG and ferromagnetic-to-SG phase transitions, in the transverse Ising SG with asymmetric bond distribution. In this paper, we shall extend this new method to study the effects of the transverse and random longitudinal fields on the instability phase boundaries and

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the multicritical point where the four phases (paraelectric, proton glass, mixed phase and ferroelectric) meet, in a deuterated RADP crystal with a Gaussian random field distribution. It will be predicted that, in the infinite-range quantum transverse Ising proton glass, the existence of a mixed phase in which the ferroelectric coexists with transverse proton glass order is likely.

We consider a system consisting of N interacting Ising spins; the Hamiltonian of the system is

$$\mathcal{H} = -\sum_{i,j} J_{ij}\sigma_i^z\sigma_j^z - \Gamma\sum_i \sigma_i^x - \sum_i H_i\sigma_i^z \tag{1}$$

where σ_i^x and σ_i^z are the Pauli matrices referred to the ith site of the lattice and Γ is a transverse field. H_i is the identically distributed random field at site i with the Gaussian probability distribution such that its average is zero and its square derivative σ^2:

$$P(H_i) = (2\pi\sigma^2)^{-1/2}\exp(-H_i^2/2\sigma^2). \tag{2}$$

The exchange coupling J_{ij} is a random Gaussian variable with mean J_0 and variance J^2:

$$P(J_{ij}) = (2\pi J^2)^{-1/2}\exp[-(J_{ij}-J_0)^2/2J^2] \tag{3}$$

where J_0 and J are scaled by

$$J_0 = \tilde{J}_0/N \qquad J = \tilde{J}/\sqrt{N} \tag{4}$$

so that $\tilde{J}_0$ and $\tilde{J}$ are intensive. The parameters σ, J and J_0 depend on the concentration x characterizing the composition of the proton glass as in the case of RADP [4, 13, 19], and the relative magnitudes of J and J_0 determine whether ferroelectric or proton-glass ordering occurs at low temperature.

Let us assume that the effective Hamiltonian for the ith spin is of the form

$$\mathcal{H}_i = -\Gamma\sigma_i^x - h_i\sigma_i^z \tag{5}$$

where h_i is the local field (including the random field H_i) at the site i. It was shown that in the infinite-range Gaussian Ising model the quenched average over the J_{ij} distribution can be replaced by the static random field [7, 18, 20], where the distribution is Gaussian with mean $\tilde{J}_0 m$ and variance $\tilde{J}^2 q$. In the present case, the local field h_i is distributed according to

$$P(h_i) = [2\pi(\sigma^2+\tilde{J}^2q)]^{-1/2}\exp[-(h_i-\tilde{J}_0m)^2/2(\sigma^2+\tilde{J}^2q)] \tag{6}$$

where m is the average magnetization and q is the static Edwards–Anderson order parameter. The corresponding one-body partition function becomes

$$Z_i = \mathrm{Tr}\,[\exp(-\beta\mathcal{H}_i)] = 2\cosh[\beta(h_i^2+\Gamma^2)^{1/2}]. \tag{7}$$

The local magnetization $m(h_i)$ and the local static transverse susceptibility $\chi(y)$ induced by the local field h_i can be given by

$$m(h_i) = (1/\beta)[\partial \ln Z_i)/\partial h_i] = h_i(h_i^2+\Gamma^2)^{-1/2}\tanh[\beta(h_i^2+\Gamma^2)^{1/2}] \tag{8}$$

$$\chi(h_i) = (\partial/\partial h_i)m(h_i) = [\Gamma^2/(h_i^2+\Gamma^2)^{3/2}]\tanh[\beta(h_i^2+\Gamma^2)^{1/2}] + [\beta h_i^2/(h_i^2+\Gamma^2)\,\mathrm{sech}^2[\beta(h_i^2+\Gamma^2)^{1/2}]. \tag{9}$$

The pair Hamiltonian in the pair approximation is given by

$$\mathcal{H}_{ij} = -J_{ij}\sigma_i^z\sigma_j^z - h_i^*\sigma_i^z - h_j^*\sigma_j^z - \Gamma(\sigma_i^x+\sigma_j^x) \tag{10}$$

where h_i^* is the local field on site i coming from other spins except from site j and equals

the one-body local field h_i in the limit of infinite interactions where every spin couples equally with every other spin. The corresponding pair partition function becomes

$$Z_{ij} = \mathrm{Tr}\,[\exp(-\beta\mathcal{H}_{ij})]. \tag{11}$$

In order to obtain the pair partition function, we shall reformulate the Hamiltonian in DPIR. The idea in DPIR is to convert the quantal two-state spin on each lattice site into a P-component vector $U(U^{(1)}, U^{(2)}, \ldots, U^{(p)})$ and eventually to let P go to infinity. Each component $U^{(t)}$ $(t = 1, 2, \ldots, p)$ is taken to be a classical two-state variable $U^{(t)} = \pm 1$, and the net effect is to represent the quantum uncertainty by creating many copies, or replicas, of the original variable. By means of the DPIR, the pair Hamiltonian can be broken up into a reference part $H_{ij}^{(0)}$ involving only the single-site terms and an interaction part V [18, 21], i.e.

$$\mathcal{H}_{ij} = \mathcal{H}_{ij}^{(0)} + V \tag{12}$$

where

$$-\beta\mathcal{H}_{ij}^{(0)} = \boldsymbol{U}_j \cdot \boldsymbol{a} \cdot \boldsymbol{U}_i + \boldsymbol{U}_j \cdot \boldsymbol{a} \cdot \boldsymbol{U}_j + \boldsymbol{h}_i \cdot \boldsymbol{U}_i + \boldsymbol{h}_j \cdot \boldsymbol{U}_j + \text{PC} \tag{13}$$

with

$$a = \tfrac{1}{2}\ln[\coth(\beta\Gamma/p)] \qquad C = \tfrac{1}{2}\ln[\cosh(\beta\Gamma/p)\sinh(\beta\Gamma/p)] \tag{14}$$

$$(\boldsymbol{a})_{t,t'} = a\delta_{t,t'-1} \qquad (\boldsymbol{a})_{p,1} = a \tag{15}$$

$$\boldsymbol{h}_i = (\beta h_i^*/p)(1, 1, \ldots, p) \tag{16}$$

$$-\beta V = (\beta J_{ij}/P)\boldsymbol{U}_i \cdot \boldsymbol{U}_j. \tag{17}$$

The free energy can be expressed in terms of the free energy F_0 of the reference part and the cumulant expansion in the reference part

$$-\beta F_{ij} = \ln\{\mathrm{Tr}[\exp(-\beta\mathcal{H}_{ij})]\} = -\beta F_0 + \sum_{n=1}^{\infty} \frac{1}{n!}(-\beta)^n C_n(V) \tag{18}$$

with

$$-\beta F_0 = \ln\{\mathrm{Tr}[\exp(-\beta\mathcal{H}_{ij}^{(0)})]\} \tag{19}$$

and the cumulants are given by

$$C_1(V) = \langle V\rangle_0,\ C_2(V) = \langle V^2\rangle_0 - \langle V\rangle_0^2, \ldots \tag{20}$$

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

$$\begin{aligned}\ln Z_{ij} = {} & \ln\{2\cosh[\beta(h_i^{*2} + \Gamma^2)^{1/2}]\} + \ln\{2\cosh[\beta(h_j^{*2} + \Gamma^2)^{1/2}]\} \\ & + \beta J_0[\{\tanh[\beta(h_i^{*2} + \Gamma^2)^{1/2}]\}/(h_i^{*2} + \Gamma^2)^{1/2}] \\ & \times h_i^*[\{\tanh[\beta(h_j^{*2} + \Gamma^2)^{1/2}]\}/(h_j^{*2} + \Gamma^2)^{1/2}]h_j^*.\end{aligned} \tag{21}$$

The free energy of the full system in the pair approximation is given by the following expression [22]:

$$-\beta F = \int P(h_i)\,\mathrm{d}h_i \int P(h_j)\,\mathrm{d}h_j \left(\sum_i \ln Z_i + \sum_{ij} (\ln Z_{ij} - \ln Z_i - \ln Z_j)\right) \tag{22}$$

where the m and q are given self-consistently by the variational equations

$$\partial F/\partial m = \partial F/\partial q = 0 \tag{23}$$

or, in other words,

$$m = \int \mathrm{d}y\,(2\pi)^{-1/2}\exp(-\tfrac{1}{2}y^2)\,m(y) = \int \mathrm{d}y\,(2\pi)^{-1/2}\exp(-\tfrac{1}{2}y^2) \times \frac{\tilde{J}_0 m + (\sigma^2+\tilde{J}^2 q)^{1/2}y}{\{(\tilde{J}_0 m + (\sigma^2+\tilde{J}^2 q)^{1/2}y]^2 + \Gamma^2\}^{1/2}} \times \tanh[\![\beta\{[\tilde{J}_0 m + (\sigma^2+\tilde{J}^2 q)^{1/2}y)^2 + \Gamma^2\}^{1/2}]\!] \tag{24}$$

$$q = \int \mathrm{d}y\,(2\pi)^{-1/2}\exp(-\tfrac{1}{2}y^2)\,m^2(y) = \int \mathrm{d}y\,(2\pi)^{-1/2}\exp(-\tfrac{1}{2}y^2) \times \frac{[\tilde{J}_0 m + (\sigma^2+\tilde{J}^2 q)^{1/2}y]^2}{\{[\tilde{J}_0 m + (\sigma^2+\tilde{J}^2 q)^{1/2}y)^2 + \Gamma^2\}} \times \tanh^2[\![\beta\{[\tilde{J}_0 m + (\sigma^2+\tilde{J}^2 q)^{1/2}y)^2 + \Gamma^2\}^{1/2}]\!]. \tag{25}$$

It is straightforward to solve equations (22)–(25) numerically for m and q and to obtain analytic results in the limiting cases.

We first consider the possibility of the SG freezing transition for $J_0 = 0$ but $\sigma \neq 0$. It is straightforward to see from equation (25) that the order parameter q remains non-zero at all temperatures, suggesting that in the presence of a Gaussian random field the SG phase transition is smeared out, i.e. the main effect of random fields is the smearing of the SG transition, which is qualitatively similar to that of the homogeneous external field.

In order to investigate the instability of the ferromagnetic phase we shall discuss the solution of equations (22)–(25) for $J_0 \neq 0$ and $\sigma = 0$. It was demonstrated that, in the Ising and Heisenberg models with random interactions, the ferromagnetic, paramagnetic and SG phases are likely. Moreover, it was shown that a mixed phase, between the SG and standard ferromagnetic phases, occurs for an asymmetric bond distribution. In particular, when $\tilde{J}_0 > \tilde{J}$ and the system is cooled from a high temperature, there is first a transition from a paramagnet to a ferromagnet and then, at a lower temperature, a second transition to a new phase which is characterized by the coexistence of ferromagnetic order and SG ordering of the transverse components of the spins. The existence of this mixed phase is implicit in the Gabay–Toulouse (GT) line. The instability boundaries between the standard ferromagnetic phase and the mixed phase M are determined from the zero point of the coefficient of the second-order term in equation (22) when the equation is expanded in terms of $q^{1/2}$. We obtain

$$\{\Gamma^2/[\Gamma^2 + (\tilde{J}_0 m)^2]^{3/2}\}\tanh\{\beta[\Gamma^2 + (\tilde{J}_0 m)^2]^{1/2}\} + \{\beta(\tilde{J}_0 m)^2/[\Gamma^2 + (\tilde{J}_0 m)^2]\}\,\mathrm{sech}^2\{\beta[\Gamma^2 + (\tilde{J}_0 m)^2]\} = 1/\tilde{J}. \tag{26}$$

The boundary between the ferromagnetic and M phases is given by the simultaneous solution of equations (24) and (26).

We now turn to locating the phase boundary between the SG phase and the mixed phase M. The SG-to-M phase transition occurs with the breakdown of the magnetization m. So the phase boundary of the SG is determined from the zero point of the coefficient of the second-order terms in equation (22) when the equation is expanded in terms of m. In the result, the second-order transition line is given by

$$\int \mathrm{d}y\,(2\pi)^{-1/2}\exp(-\tfrac{1}{2}y^2)\left(\frac{\Gamma^2}{[\Gamma^2 + (\sigma^2+\tilde{J}^2 q)y^2]^{3/2}}\tanh\{\beta[\Gamma^2 + (\sigma^2+\tilde{J}^2 q)y^2]^{1/2}\} + \frac{\beta(\sigma^2+\tilde{J}^2 q)y^2}{\Gamma^2 + (\sigma^2+\tilde{J}^2 q)y^2}\,\mathrm{sech}^2\{\beta[\Gamma^2 + (\sigma^2+\tilde{J}^2 q)y^2]^{1/2}\}\right) = \frac{1}{\tilde{J}_0}. \tag{27}$$

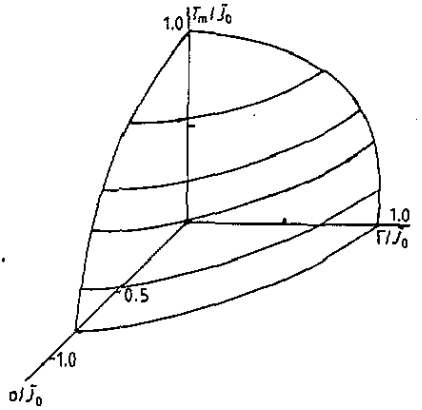

Figure 1. The multicritical temperature T_m as a function of the transverse field Γ and Gaussian random field variance σ.

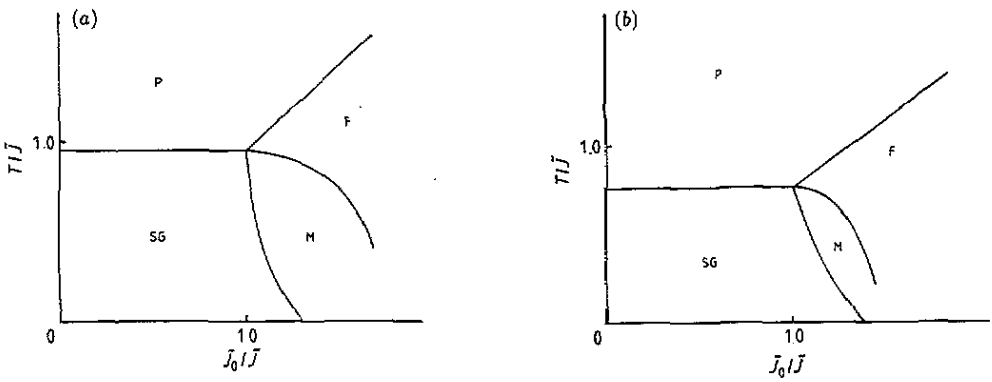

Figure 2. Phase diagrams of the quantum infinite-range SG model with non-zero mean J_0 in the distribution, for two values of transverse field Γ: (*a*) $\Gamma/\tilde{J} = 0.25$; (*b*) $\Gamma/\tilde{J} = 0.75$. The phases are paramagnetic (P), spin glass (SG), ferromagnetic (F)—and a mixed phase (M) in which ferromagnetism coexists with transverse SG order.

The boundary between the SG and M phases is given by the simultaneous solution of equations (25) and (27). It is easy to see that the transverse and random fields make the M-phase ordering unstable separately, and even the phase boundaries of the M phase can be smeared out, which depends strongly on the values of $\sigma/\tilde{J}_0$ or $\Gamma/\tilde{J}_0$. On the other hand, it is clear on physical grounds that the boundary between the paramagnetic and ferromagnetic phase is obtained by solving equation (27) where $q = 0$, and the result of the non-random Ising model in a transverse and a Gaussian random field can be derived from the present formula for $J \to 0$ [23]. A multicritical point occurs at $\tilde{J} = \tilde{J}_0$, which is determined by simultaneous solution of equations (26) and (27). Figure 1 shows the dependence of the multicritical temperatures on the transverse and random longitudinal fields. As is seen from this figure, the multicritical points are lowered on increase in the strength of the random field and transverse field separately, until it reaches $T = 0$ for $\sigma/\tilde{J}_0 = \sqrt{2}/\pi$ or $\Gamma/\tilde{J} = 1$. Finally, in figure 2 we illustrate the changes in the phase diagrams for differing values of the transverse field Γ when $J_0 \neq 0$ and $\sigma = 0$. It should be noted that quantum fluctuations have the effect of destroying the ordering phase, until the M-phase ordering disappears for $\Gamma = \tilde{J}_0$. This result may help to explain the existence of a

mixed phase in which the ferroelectric phase coexists with transverse proton-glass order in some recent experimental findings [24].

In conclusion, we have used a new method, which combines the pair approximation with the DPIR, to perform the instability analysis of the infinite-range Ising SG model with a transverse and a Gaussian random field. We see that, in the presence of the transverse field, long-range ferromagnetic order can indeed coexist with SG order, owing to freezing of the spin components transverse to the applied field and the ordering regions are suppressed by the existence of both quantum fluctuations and randomness. It will be interesting to study the instability boundaries of the replica-symmetry solution which is analogous to the de Almeida–Thouless line for an Ising system in a longitudinal field by use of the present method [25]. These are projects for further investigation.

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