Ising spin glass in a transverse magnetic field

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We study the three-dimensional quantum Ising spin glass in a transverse magnetic field following the evolution of the bond probability distribution under renormalization-group transformations. The phase diagram (critical temperature T_c vs transverse field Γ) we obtain shows a finite slope near $T = 0$, in contrast with the infinite slope for the pure case. Our results compare very well with the experimental data recently obtained for the dipolar Ising spin glass $LiHo_{0.167}Y_{0.833}F_4$, in a transverse field. This indicates that this system is more appropriately described by a model with short-range interactions than by an equivalent Sherrington-Kirkpatrick model in a transverse field.

The role of quantum fluctuations in spin glasses has been a long standing theoretical problem.[1–3] The so-called proton glasses[4–6] — a random mixture of ferroelectric and antiferroelectric materials such as $Rb_{1-x}(NH_4)_xH_2PO_4$ — provide an experimental realization for quantum spin glasses. Within a pseudospin description of such hydrogen-bonded systems, the proton position in the two potential minima is represented by Ising states, $\sigma^z = \pm 1$, and the tunneling between the minima by a transverse field term, $\Gamma\sigma^x$, where Γ is the tunneling frequency.[7] The theoretical study of Ising spin glasses in a transverse field (TISG) has then attracted renewed interest, especially in relation to the analog of the Sherrington-Kirkpatrick model[8] in a transverse field (TSK); see, e.g., Ref. 9 and references therein. More recently, the magnetic susceptibility of the (long-ranged dipolar) Ising spin glass $LiHo_{0.167}Y_{0.833}F_4$ has been measured in the presence of a transverse field H_t, from which a phase diagram $T_c(H_t)$ was determined.[10,11] Therefore, it is of interest to discuss the main differences between the phase diagrams of the transverse Ising model in both pure and spin-glass cases. In view of the long-range nature of the interactions in the dipolar glass, we are also particularly interested in establishing whether this system can be suitably described by a short-range model or one has to resort to the TSK model. Here we address these questions using real-space scaling methods.

The TISG model is described by the Hamiltonian

$$-\beta\mathcal{H} = \sum_{i<j}^{N} J_{ij}\sigma_i^z\sigma_j^z + \Gamma\sum_i^N \sigma_i^x, \qquad (1)$$

where the σ_i^μ, $\mu = x,z$ are Pauli spin matrices, Γ is the transverse field, i and j are nearest-neighbor sites on a simple cubic lattice, and the J_{ij} are uncorrelated exchange couplings chosen at random from an even distribution. For zero transverse field the model reduces to the classical Ising spin glass, and quantum effects are brought in by increasing the field. At finite temperatures, the effect of the transverse field is to depress the

spin-glass transition temperature, whereas at zero temperature quantum fluctuations are the only mechanism driving the system to a phase transition at a critical value of the transverse field. It is interesting to note that the lower critical dimension (d_ℓ) for zero-temperature transitions in the transverse Ising spin-glass model is[3] $d_\ell < 1$, unlike the classical Ising case,[12] $d_\ell = 2$.

In the context of real-space renormalization group, the simple cubic lattice may be approximated by hierarchical Migdal-Kadanoff cells;[13] see Fig. 1. The terminal sites are connected by b^{d-1} bonds "in parallel," each of which consists of b bonds "in series"; b is the scaling factor ($b = 2$ in Fig. 1) and d is the space dimensionality of the lattice ($d = 3$ in this case). For the transverse Ising model (TIM), the noncommutation aspects are present at the cluster level, in the sense that individual spins are not in a definite state. This can be dealt with by referring the density matrix to the basis $|m_1 m_2 \cdots m_N\rangle$, where $\sigma_i^z|m_i\rangle = m_i|m_i\rangle$, and defining the renormalization-group transformation (RGT) by the mapping of diagonal elements only. This approach has been successfully used in a detailed study of the pure and bond-diluted TIM in two dimensions.[14] In the present work bond disorder is included within a statistical renor-
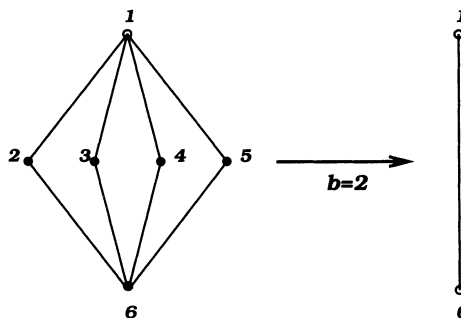

FIG. 1. Clusters used in the RG transformation in three dimensions. The terminal sites are labeled 1 and 6.

malization group (SRG) treatment: one follows the effect of a RGT on the probability distributions of the relevant parameters, instead of forcing them into a particular form.[15] Several aspects of the Ising spin glass[16] and of the random field Ising model[17] have been elucidated by treating disorder this way.

Thus, for a given bond configuration ($\{J_{ij}\}$), an RGT

for the $d = 3$ system (Fig. 1) is defined by

$$\langle m_1 m_6 | \rho'(\mathbf{K}') | m_1 m_6 \rangle = \langle m_1 m_6 | \tilde{\rho}(\mathbf{K}) | m_1 m_6 \rangle, \qquad (2)$$

where $\mathbf{K}' = (J', \Gamma', C')$ are the renormalized quantities in the two-site cell, $\mathbf{K} = (\{J_{ij}\}, \Gamma)$ refers to the original cluster, and

$$\langle m_1 m_6 | \tilde{\rho}(\mathbf{K}) | m_1 m_6 \rangle = \sum_{m_2 m_3 m_4 m_5} \langle m_1 m_2 m_3 m_4 m_5 m_6 | \rho(\mathbf{K}) | m_1 m_2 m_3 m_4 m_5 m_6 \rangle \qquad (3)$$

is obtained by performing the partial trace on the internal spins, keeping those on the terminal sites fixed (see Fig. 1). The third matching condition required to solve the problem for the three unknowns (J', Γ', C') is obtained by preserving the thermodynamical average of the rotation operator

$$\langle \sigma_1^x \sigma_6^x \rangle_{\mathcal{H}'} = \langle \sigma_1^x \sigma_2^x \sigma_3^x \sigma_4^x \sigma_5^x \sigma_6^x \rangle_{\mathcal{H}'}. \qquad (4)$$

For the renormalized cell, Eqs. (3) and (4) provide analytical expressions for the three primed unknown variables.[14] Since disorder destroys the point group symmetry of the original cluster, the Hamiltonian matrix is written in a 64×64 representation and Eqs. (3) and (4) are calculated numerically. At this point we should comment that a single renormalized field appears in the recursion relations as a result of the approximation employed here: the fields are assumed to be uniform in both renormalized and original cells. This assumption can be justified, to some extent, by recalling that the transverse magnetic field behaves as an irrelevant variable in the pure TIM. Since the transverse field is not a symmetry breaking operator, this should hold in the spin-glass case as well. On the other hand, we could have allowed the field at each site to follow an RG trajectory. The irrelevance of the field would manifest itself through a distribution evolving from an initial δ function centered at $\Gamma = \Gamma_0$ into one centered at $\Gamma = 0$.

The initial probability distribution for the exchange couplings is

$$P(J_i) = \frac{1}{\sqrt{2\pi \tilde{J}^2}} \exp\left[-\frac{J_i^2}{2\tilde{J}^2}\right], \qquad (5)$$

where we have assigned an index i to each bond in the original cell and taken $\langle J_i J_l \rangle = \tilde{J}^2 \delta_{il}$ and $\langle J_i \rangle = 0$. We start the iteration by choosing eight bonds distributed according to Eq. (5) and one value of the transverse field $[P(\Gamma) = \delta(\Gamma_i - \Gamma)]$, to feed the recursion relations and generate a new value of the field and of the exchange coupling. This procedure is repeated about 10 000 times and we obtain two renormalized distributions, $P'(J_i')$ and $P'(\Gamma')$. We make use of these distributions to feed the recursion relations in the next step of the renormalization process: eight bonds and one field are chosen according to the new distributions, and this is done again 10 000 times. The evolution of the distributions is then followed along the renormalization process. We find that the bond

probability distribution remains symmetric around $J = 0$ at each iteration; that is, $\langle J_{ij} \rangle = 0$. The attractors of the different phases are determined by fixed distributions characterized by their width $\tilde{J}$ and mean value $\langle \Gamma \rangle$, as follows:

$$\tilde{J} \to \infty, \quad \langle \Gamma \rangle \to 0 \quad \text{spin glass},$$

$$\tilde{J} \to 0, \quad \langle \Gamma \rangle \to 0 \quad \text{paramagnetic},$$

so that the critical curve is determined as the boundary between these two different behaviors. Note that in every case the average value of the transverse field distribution iterates to zero.

In Fig. 2 we present our results for the phase diagram, T_c vs Γ, for both pure and spin-glass cases. For comparison we also display the spin-glass data for the replica-symmetry-breaking (RSB) solution of the TSK model,[9] and for LiHo$_{0.167}$Y$_{0.833}$F$_4$.[10,11] In analyzing the experimental data one should have in mind[10,11] that the applied transverse field H_t gives rise to a level splitting $\sim H_t^2$ (at low fields) which, in the context of Eq. (1), is proportional to Γ; thus, $\Gamma \sim H_t^2$. For the pure TIM, the critical line both for small fields and near $T = 0$ has a square fit: $T_c(0) - T_c(\Gamma) \sim \Gamma^2$ and $\Gamma_c(T) - \Gamma_c(0) \sim T^2$, respectively. Still for the pure case, the critical field for zero-temperature transitions obtained with the present RG is $(\Gamma/J)_c = 3.40$, which should be compared with the series result,[18] $(\Gamma/J)_c = 5.14$; similarly, our result
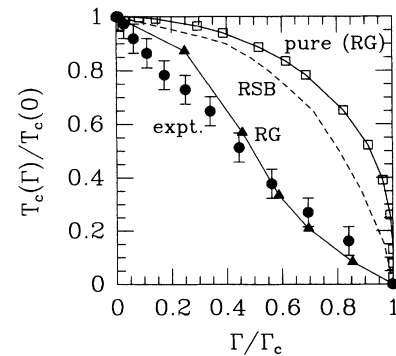

FIG. 2. Critical temperature vs transverse field for the Ising model. ($\square$) and ($\blacktriangle$) denote our renormalization group (RG) results in the pure and spin-glass cases, respectively. The replica-symmetry-breaking (RSB, Ref. 9) results (— — —) and the experimental data ($\bullet$) for LiHo$_{0.167}$Y$_{0.833}$F$_4$ (Refs. 10 and 11) are also shown.

$T_c(0) = 3.83J$ should be compared with $T_c = 1.13J$, obtained from series expansions for the three-dimensional Ising model.[19] As usual, the critical parameters obtained within a simple Migdal-Kadanoff approximation are quite inaccurate, but one is generally able to describe the qualitative aspects of phase diagrams.[13,15]

For the transverse Ising spin glass, we obtain a curve $T_c(\Gamma)$ with a finite slope near $T = 0$, unlike both the pure case and the replica-symmetry-breaking solution to the TSK model; see Fig. 2. Overall, the experimental data are better represented by the present approach than by the infinite-range mean-field model.[9] This can be explained by the fact that in the actual crystal, the dipolar interactions fall off with the distance, being effectively reduced to zero for distances greater than a few lattice spacings. In contrast, the interactions between any pair of spins in the mean-field model have the same intensity, irrespective of the distance between them. The calculated critical parameters in this case are: $\Gamma_c = 1.58J$ at $T = 0$ and $T_c = 0.884J$ at zero transverse field. In agreement with the experimental results[10,11] we find that temperature is more effective in destroying the spin-glass order than quantum fluctuations.

We point out that the renormalization-group trajectory along the critical line flows away from the zero-temperature fixed point, towards the one controlling the classical finite-temperature spin-glass transition. This has two main implications:

(1) The shape of the critical line close to $\Gamma = 0$ is analytic.[20] In the present case our results are consistent with $T_c(0) - T_c(\Gamma) \sim \Gamma^2$.

(2) The exponents controlling the transition for finite Γ are the same as those of the classical spin-glass transition, except at zero temperature where quantum effects become dominant.

We can develop a scaling theory for the spin-glass transition close to the unstable zero-temperature fixed point at $(\Gamma/J) \simeq (\Gamma/J)_c$. Introducing an exponent z through the scaling relation[21]

$$\tilde{J}' = b^{-z}\tilde{J}, \qquad (6)$$

we obtain the scaling form for the free energy density close to $(\Gamma/J)_c$ as[21]

$$f = |g|^{2-\alpha} \mathcal{F}\left[\frac{(T/J)}{|g|^{\nu z}}\right], \qquad (7)$$

where $g = |(\Gamma/J) - (\Gamma/J)_c|$, ν and z are the correlation length and the dynamic exponents, respectively, and α is a critical exponent which describes the singularity of the ground-state energy; all these exponents are associated with the zero-temperature fixed point and are related through the modified hyperscaling relation $2 - \alpha = \nu(d + z)$. Close to $(\Gamma/J) \simeq (\Gamma/J)_c$ the critical temperature vanishes as

$$T_c \propto |g|^{\nu z}, \qquad (8)$$

which allows us to obtain the product νz. Our RG results for the behavior of the phase boundary near $T = 0$ yield $\nu z \simeq 1.23$. An independent calculation of the exponent z through a finite size scaling analysis[22] for the gap at the critical point yields $z = 1.40$. Using these results we obtain $\nu = 0.87$ consistent with the exact constraint $\nu \geq 2/d$ for disordered systems.[23] The finite slope of the phase boundary close to $T = 0$ is a consequence of the fact that $\nu z > 1$ for the disordered case differently from the pure three-dimensional case where $\nu z = 1/2 < 1$.

In conclusion, we have examined the phase diagram of the transverse Ising spin glass model. We have compared our data with those obtained experimentally for the dipolar Ising spin glass $LiHo_{0.167}Y_{0.833}F_4$ with an applied field in the transverse direction. In spite of the long-range character of the interactions between spins, this system is more appropriately described by a model with short-range interactions than by the equivalent Sherrington-Kirkpatrick model in a transverse field.[9] However, the small value of the exponent γ associated with the nonlinear susceptibility was found experimentally[11] to be quite different from that of the classical spin-glass transition. This remains a puzzle from the point of view of our results. Further theoretical and experimental studies are required to clear this point. Work is in progress to investigate the possibility of the transition at $T = 0$ being first order, and to obtain a more detailed scaling analysis of this transition.

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