Scaling theory for the quantum spin-glass transition

M. A. Continentino
Instituto de Física, Universidade Federal Fluminense, Outeiro de São João Batista, s/n, 24210 Niterói, Brazil

Beatriz Boechat* and Raimundo R. dos Santos*†
Departamento de Física, Pontifícia Universidade Católica do Rio de Janeiro, Caixa Postal 38071, 22452-970 Rio de Janeiro, Brazil

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We present a scaling theory for the low-temperature phase transition of the Ising spin glass in a transverse magnetic field (Γ). The theory provides relations and bounds on some critical exponents, which are supported by results from actual calculations. A renormalization-group analysis of the zero-temperature transition in the presence of a longitudinal symmetry-breaking field enables us to estimate the critical exponents β and γ, associated with the Edwards-Anderson order parameter and the nonlinear susceptibility, respectively. We have found no indications of the transition being of first order.

The interest in quantum spin glasses[1–3] has been renewed over the past years, from both theoretical and experimental points of view. In particular, the first systematic measurements of quantum effects, carried out[4,5] in the three-dimensional dipolar Ising spin glass $LiHo_{0.167}Y_{0.833}F_4$ by varying the intensity of a transverse magnetic field Γ, stimulated further theoretical studies of the transverse Ising spin glass (TISG).[6–8] One feature emerging from magnetic susceptibility data[4,5] is that the critical curve displays a *linear* dependence of T_c with Γ; see Fig. 1. This should be contrasted with the theoretical results for the Sherrington-Kirkpatrick model in a transverse field (see, e.g., Ref. 9 for a list of references), according to which $T_c(\Gamma)$ should have an infinite slope at small temperatures for $\Gamma = \Gamma_c$, similarly to the pure case. In the pure case this can be traced back to the fact that the gap for excitations is finite (usual discrete Ising symmetry) for any $\Gamma < \Gamma_c$; that is, one needs a finite thermal energy to overcome the gap and destroy the transition even for $\Gamma = \Gamma_c^-$. Conversely, the finite slope found in the experimental phase diagram for the spin glass[4,5] can be attributed to a vanishing configurationally averaged gap for $\Gamma \leq \Gamma_c$. We have recently examined a short-ranged TISG model in three dimensions by real-space renormalization-group (RSRG) methods,[6] and found very good qualitative agreement with the experimental phase diagram, including the finite slope at the zero-temperature critical field, Γ_c; see Fig. 1. This is indicative that a short-range model provides a better description of $LiHo_{0.167}Y_{0.833}F_4$ than its infinite range counterpart.

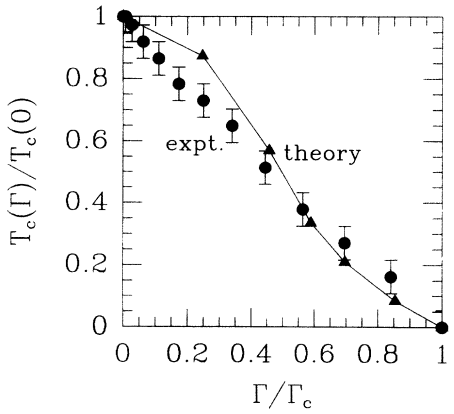

FIG. 1. Critical temperature for the Ising spin glass in a transverse field; J is the exchange coupling, as it appears in Eq. (1). Our previous renormalization-group results (▲, Ref. 6) are compared with the experimental data for $LiHo_{0.167}Y_{0.833}F_4$ (•, Refs. 4 and 5).

A second feature emerging from the experimental analysis concerns the behavior of the nonlinear susceptibility[5] as the critical curve is approached. It diverges in the classical regime (i.e., small transverse fields; see Fig. 1), with a critical exponent $\gamma \simeq 0.2$, but is suppressed at very low temperatures (the quantum regime). The measured γ is quite smaller than typical (both experimental and theoretical) values for classical spin glasses,[10] for which $\gamma \sim 2.5$. Wu *et al.*[5] attribute this unusual behavior of the nonlinear susceptibility to the nature of the $T = 0$ transition, which could be of first order. This is in disagreement with theoretical expectations,[6] since the renormalization group-trajectory along the critical line flows towards the thermal fixed point [i.e., $T = T_c(0)$] of the classical three-dimensional spin glass. Thus, all exponents controlling the transitions at finite temperatures and transverse magnetic fields should be the same as those of the (classical) Ising spin-glass transition. To clarify this point, a detailed study of the zero-temperature transition is surely in order, and here we present the scaling theory near the transition at $(\Gamma/J) = (\Gamma/J)_c$; this is complementary to recent Monte Carlo simulations for the TISG at zero temperature in two[7] and three dimensions.[8]

For a complete scaling analysis, including the discussion of the order of the transition, we must introduce a symmetry-breaking longitudinal magnetic field. However, due to the nature of the Edwards-Anderson order parameter,[10] the local longitudinal fields H_i are also ran-

dom variables distributed according to an even probability distribution $P(H_i)$; the field conjugate to the spin-glass order parameter is therefore defined[10] as the width of $P(H_i)$,

$$h_L = \sqrt{[H^2]}, \tag{1}$$

where $[\cdots]$ denotes a configurational average. The transverse Ising Hamiltonian then becomes

$$-\beta\mathcal{H} = \sum_{i<j}^{N} J_{ij}\sigma_i^z\sigma_j^z + \Gamma\sum_i^N \sigma_i^x + \sum_i^N H_i\sigma_i^z, \tag{2}$$

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 J_{ij} are uncorrelated exchange couplings chosen at random from an even distribution.

Defining $J = \sqrt{[J^2]}$, where $[J^2]$ is the second moment of the $P(J_{ij})$ bond probability distribution, the renormalization of J and Γ near the unstable zero-temperature fixed point is described in terms of the variable $g = (\Gamma/J) - (\Gamma/J)_c$, which measures the distance to the critical point. One has[11,12]

$$g' = b^{1/\nu} g\ , \tag{3}$$

where, in standard notation, ν is the correlation length exponent for the zero-temperature transition. In the TISG problem the renormalized temperature behaves as a relevant field and scales as[6,12]

$$\left(\frac{T}{J}\right)' = b^z \left(\frac{T}{J}\right), \tag{4}$$

near $T = 0$, and z is the dynamical critical exponent,[12] which should not be confused with the ordinary model A dynamical exponent.[13]

With Eqs. (3) and (4) we can discuss the scaling functions in the so-called extended form.[14] For example, the free energy density close to $(\Gamma/J)_c$ is

$$f = |g|^{2-\alpha}\,\mathcal{F}_0\left[\frac{(T/J)}{|g|^{\phi_T}}\right], \tag{5}$$

where

$$\phi_T \equiv \nu z \tag{6}$$

is the exponent describing the crossover induced by the temperature field, and one should note the use of the *unshifted* variable g in Eq. (5). The function $\mathcal{F}_0(x = 0)$ has a constant value such that the exponent α is associated with the singularity of the ground state energy density at the $T = 0$ transition. The shape of the critical curve at low temperatures is given by

$$T_c \sim |g|^{\psi}\ , \tag{7}$$

defining the shift exponent ψ. Therefore, the crossover temperature $T^\times$, as given by the invariance of the scaling variable in Eq. (5), is proportional to the critical temperature in this case, and one has, necessarily,[14]

$$\psi = \phi_T = \nu z. \tag{8}$$

Alternatively, one may consider a scaling form in terms of the *shifted* variable,

$$\dot{g} = \lambda - \lambda_c(T);\ \lambda \equiv \Gamma/J, \tag{9}$$

as

$$f = |\dot{g}|^{2-\alpha}\,\mathcal{F}\left[\frac{(T/J)}{|\dot{g}|^{\phi_T}}\right]. \tag{10}$$

Inverting Eq. (7) gives $\lambda_c(T) = \lambda_c(0) + A\ T^{1/\psi}$, where A is a nonuniversal amplitude. In this case, $(T/J)'$ in Eq. (4) should also depend on g,[11,12] and so the invariance of the scaling variable in (10) defines the crossover temperature as

$$T^\times \sim \begin{cases} g^{\psi} & \text{if } \psi \geq \phi_T\ , \\ g^{\phi_T} & \text{if } \psi \leq \phi_T\ . \end{cases} \tag{11}$$

This implies that the shift and crossover exponents are not related in principle, and the former should be determined independently. Nevertheless, the analyticity of the renormalization-group equations in this case demands that ψ^{-1} be an integer (usually 1 or 2).[12] At this point it is worth mentioning that the choice between the usual and extended forms is not obvious *a priori*. An exact RG treatment would, in principle, select one of them, since the form (10) would arise from the coupling of the two competing variables (e.g., T and g in our case) under a change in length scale. In the absence of exact results, however, one has to adopt a different strategy, collecting as much information as possible, especially the shift exponent ψ, which can, in principle, be estimated directly from the shape of the phase boundary. If $\psi = \phi_T$, both scaling forms are equivalent and the final choice is dictated by a mere convenience; if, on the other hand, $\psi \neq \phi_T$, then Eq. (10) is the apropriate scaling form. With a few notably exceptions (see below), the equality $\psi = \phi_T$ seems to be satisfied for the majority of crossover phenomena, especially in disordered systems.

We recall that all exponents appearing so far are associated with the zero-temperature fixed point, where quantum fluctuations replace thermal ones. As a result, the spatial dimensionality d in the scaling laws is replaced by $d + z$; see, e.g., Ref. 15. For instance, the hyperscaling relation becomes

$$(d + z)\nu = 2 - \alpha. \tag{12}$$

Let us first discuss the scaling for the *pure* transverse Ising model (TIM), in which case configurational averages are absent. The critical behavior at zero temperature is the same as that of the $(d+1)$-dimensional classical Ising model,[16] and we have $z = 1$, so that $\phi_T = \nu$. In addition, a scaling analysis[17] suggests that $\psi = 1/2 < \phi_T \simeq 0.63$ in two dimensions, and $\psi = \phi_T = 1/2$ in three dimensions.

In the presence of disorder, the equivalent classical sys-

tem corresponds to d-dimensional hyperplanes with the *same* disorder configuration; these hyperplanes are coupled through nonrandom coupling constants along the "time" direction,[16] just like in the pure case. Due to this constraint, it is no longer true that the disordered TIM at $T = 0$ is equivalent to a $d+1$ *uncorrelated* classical disordered Ising model. Because of this, time (τ) and space do not scale proportionally to each other, but to a power: $\xi_\tau \sim \xi^z$. As mentioned before, spin-glass disorder wipes out the effective excitation gap, suggesting a behavior similar to systems with continuous symmetry, at least as far as indicating that one should expect $z > 1$.[15,18] Indeed, in Ref. 6 we estimated $z \simeq 1.4$, consistent with this inequality and with Monte Carlo results, $z = 1.5 \pm 0.05$ and $z \sim 1.3$ in two and three dimensions, respectively.[7,8] It is interesting to notice that, unlike the pure case, z seems to be dependent on the dimensionality. Equation (8) then yields

$$\psi = \phi_T > 2/d, \tag{13}$$

where we have used the rigorous inequality $\nu \geq 2/d$.[19] In order to test these bounds, we recall our previous estimate,[6] $\psi \simeq 1.23$, as determined directly from the critical curve. With the above value for z, one then has $\nu \simeq 0.87$, which also compares very well with $\nu \simeq 0.8$, obtained from Monte Carlo simulations.[8] The bounds (13) are clearly satisfied for $d = 3$. For the sake of completeness, it is also worth noting that, in two dimensions, a Migdal-Kadanoff approximation at zero temperature[3] yields $\nu = 1.0$, in excellent agreement with Monte Carlo simulations,[7] $\nu = 1.0 \pm 0.1$. On the other hand, if one scales with the shifted variable as in Eq. (10), the value $\psi = 1$ seems to be the appropriate one, satisfying both the experimental data and the analyticity requirement;[12] the discrepancy with the value $\psi \simeq 1.23$, obtained from the RSRG method, should be attributed to finite-size effects. If one further assumes the equality $\phi_T = \psi = 1$ to hold, the bounds (13) are still satisfied and we could use our result[6] $z \simeq 1.4$ to estimate $\nu = \psi/z \simeq 0.71$; in this case, the error of about 10% relative to ν obtained from Monte Carlo simulations is also acceptable in the context of RG approximations. In principle, the exponent ν could be calculated independently from the recursion relations at zero temperature, which we were unable to do in a reliable way due to rounding numerical errors. To sum up this discussion, our estimates for critical exponents are consistent with both scaling forms, and so they cannot be used to single out either of them.

In order to obtain a scaling form for quantities such as the order parameter or the susceptibility it is necessary to introduce a new exponent θ, associated with the scaling of the field conjugate to the order parameter close to the unstable fixed point,

$$h'_L = b^\theta h_L. \tag{14}$$

The connection with the nonzero-temperature scaling theory of spin glasses is achieved by taking $h_L \propto h_{\rm ext}^2$, where $h_{\rm ext}$ is the applied external uniform longitudinal magnetic field.[20]

The invariant form of the longitudinal-field-dependent ground state energy is given by

$$E = |g|^{2-\alpha}\, \mathcal{F}_1 \left[\frac{(h_L/\Gamma)}{|g|^{\phi_H}} \right], \tag{15}$$

with

$$\phi_H \equiv \nu(\theta + z), \tag{16}$$

in terms of which the Edwards-Anderson spin-glass order parameter q is calculated as[10]

$$q = \frac{\partial E}{\partial h_L} = |g|^{2-\alpha-\phi_H} \equiv |g|^\beta . \tag{17}$$

Using Eq. (12), one has

$$\beta = \nu(d - \theta). \tag{18}$$

Similarly, we obtain the nonlinear susceptibility as

$$\chi_2 = \frac{\partial^2 E}{\partial h_L^2} = |g|^{2-\alpha-2\phi_H} \equiv |g|^{-\gamma} . \tag{19}$$

Alternatively, as one lowers the temperature with $(\Gamma/J) = (\Gamma/J)_c$, the nonlinear susceptibility diverges as $\chi_2 \sim T^{-\gamma/\nu z}$; see Ref. 12. This is a very useful result in the sense that the ratio $\gamma/\nu z$ can be directly measured experimentally.

Equation (19) allows one to relate γ with θ:

$$\gamma = \nu(2\theta + z - d), \tag{20}$$

and it is easy to check that the exponents α, β, and γ associated with the zero-temperature transition are related through the usual scaling law $\alpha + 2\beta + \gamma = 2$.

If the zero-temperature transition is of first order, the scaling exponent associated with the field conjugate to the order parameter, h_L, is equal to the dimension of the system,[21] i.e., $\theta = d$. In this case we would have

$$\gamma = \nu(d + z) \quad \text{and} \quad \beta = 0. \tag{21}$$

Note that in general one has $\gamma \leq \nu(d + z)$, since for a second-order transition $\theta < d$.

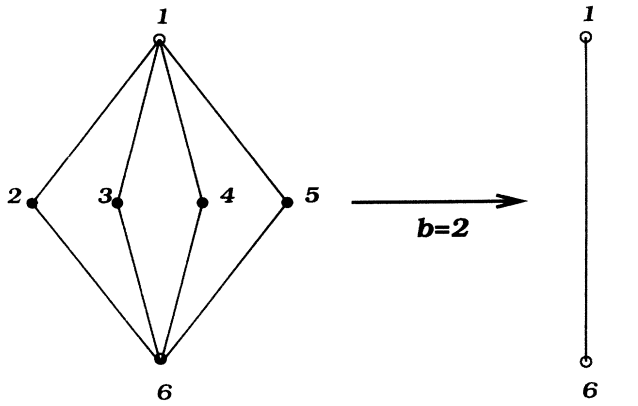

FIG. 2. Clusters used in the RG transformation in three dimensions. The terminal sites are labeled 1 and 6.

We can obtain estimates for the magnetic exponents ϕ_H from a RSRG calculation along the lines described in Ref. 6, using the hierarchical Migdal-Kadanoff cells[22] shown in Fig. 2. At zero temperature, the density matrix becomes the ground state projector, which is nondiagonal in the basis $|m_1 m_2 \cdots m_N\rangle$, where $\sigma_i^z|m_i\rangle = m_i|m_i\rangle$. Within a diagonal aproximation,[11] the projector is referred to the $|m_1 m_2 \cdots m_N\rangle$ basis, and the RSRG transformation is defined by the mapping of diagonal elements only; in spite of this truncation, quantum effects are being taken care of.[11] Further, disorder is incorporated through a statistical RSRG treatment; i.e., one follows the evolution of the full probability distributions of the parameters in the Hamiltonian,[6] Eq. (2). For a given disorder configuration, the RSRG transformation for the clusters in Fig. 2 is defined by

$$\langle m_1 m_6|\rho'(\mathbf{K}')|m_1 m_6\rangle = \langle m_1 m_6|\tilde{\rho}(\mathbf{K})|m_1 m_6\rangle, \qquad (22)$$

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

$$\langle m_1 m_6|\tilde{\rho}(\mathbf{K})|m_1 m_6\rangle = \sum_{m_2 m_3 m_4 m_5} \langle m_1 m_2 m_3 m_4 m_5 m_6|\rho(\mathbf{K})|m_1 m_2 m_3 m_4 m_5 m_6\rangle \qquad (23)$$

is obtained by performing the partial trace on the internal spins, keeping those on the terminal sites fixed (see Fig. 2). We recall that ρ in the above equations should be understood as a ground state projector.

Equation (22) provides all matching conditions required to solve the problem in the zero-temperature limit. We have obtained approximate recursion relations, calculating the corrections for the Hamiltonian eigenvalues and eigenvectors up to second order in the field H, since we are interested in the limit $H \to 0$. We considered zero-mean Gaussian probability distributions for both the local fields,

$$P(H_i) = \frac{1}{\sqrt{2\pi h_L^2}} \exp\left[-\frac{H_i^2}{2h_L^2}\right], \qquad (24)$$

and for the exchange couplings,

$$P(J_{ij}/\Gamma) = \frac{1}{\sqrt{2\pi \tilde{J}^2}} \exp\left[-\frac{(J_{ij}/\Gamma)^2}{2\tilde{J}^2}\right], \qquad (25)$$

where $\tilde{J} \equiv (J/\Gamma)_c$ is the critical width and we took $h_L \sim 10^{-5}$. When dealing with disordered magnetic fields, one must consider the total field acting on a spin on a given site as being a sum of n fields, where n is the coordination number of that site.[23] Thus, to perform the iteration we choose at random 8 bonds and 16 magnetic fields (see Fig. 2), according to Eqs. (25) and (24), respectively. The scaling exponent θ is defined through Eq. (14) and we obtain $\theta = 1.46$. Taking into account our previous estimates, $z \simeq 1.4$ and $\nu \simeq 0.87$, one has $\phi_H = 2.5$, $\beta = 1.34$, and $\gamma = 1.16$. The latter is much smaller than the upper bound $\gamma = 3.83$, which would be expected for a first order transition, as predicted in Eq. (21); evidently, the same conclusion can be drawn if the values for z and ν used were those from Monte Carlo simulations.[8] Thus, a second-order transition is more likely in this case, with the exponent for the nonlinear susceptibility being about half of the classical value.[10]

In summary, we presented a scaling theory for the three-dimensional Ising spin glass in a transverse field near zero temperature, from which bounds on critical exponents and relations among them were established. In particular, our renormalization-group estimates satisfy the available bounds and indicate that the zero-temperature spin-glass transition is of second order. In view of this, an alternative explanation for the experimentally observed suppression of the nonlinear susceptibility at low temperatures should be sought.

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* Present address: Instituto de Física, Universidade Federal Fluminense, Outeiro de São João Batista, s/n, 24210 Niterói, Brazil.
† Electronic address: rrds@fis.puc-rio.br

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