Zero-Temperature Critical Behavior of the Infinite-Range Quantum Ising Spin Glass

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We examine the *quantum* phase transition at zero temperature between paramagnetic and spin-glass-ordered phases as the strength of a uniform transverse field, Γ, is varied. At the critical point, Γ_c, the spin autocorrelation function decays with time, t, as t^{-2}. As the transition is approached from the paramagnetic phase the nonlinear susceptibility diverges as $\{|\ln(\Gamma-\Gamma_c)|/(\Gamma-\Gamma_c)\}^{1/2}$.

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Spin glasses consist of magnetic spins that are placed randomly in a material. The resulting interactions between the spins are sufficiently random that the low-temperature equilibrium state of the material exhibits no ferromagnetic or antiferromagnetic long-range order in any spatially periodic pattern. Nevertheless, the material may have a spin-glass-ordered phase where it exhibits magnetic long-range order in an aperiodic, sample-specific random pattern. The continuous phase transition between this spin-glass phase at low temperatures and the *disordered*, paramagnetic phase at higher temperatures is driven by thermal fluctuations. When this transition occurs at nonzero temperature, quantum fluctuations are unimportant in determining the critical behavior. For Ising spins in d-dimensional space, the nature of this thermally driven phase transition and its critical exponents are known to fair accuracy from experimental, theoretical, and numerical studies [1].

The spin-glass-ordered ground state may also be destabilized by quantum fluctuations [2]. As one varies the strength of the quantum fluctuations there can be a phase transition at zero temperature between spin-glass ordered and *disordered* ground states. This quantum phase transition has received less attention and is the subject of this paper. The strength of the quantum fluctuations can be adjusted, for example, by changing the relative concentration of magnetic spins and itinerant electrons in a Kondo-like system, or, more simply, by applying a transverse magnetic field to an Ising system, as is done in the recent study of $LiHo_{0.167}Y_{0.833}F_4$ [3]. Here we consider a model Ising spin glass in a transverse magnetic field.

The locations of the zero-temperature phase transitions of the quantum Ising spin glass, in a transverse field on a linear chain ($d=1$), were worked out years ago [4]. The spin-spin interactions are not frustrated in this model, so it may miss some of the essential physics of real spin glasses. Nevertheless, it has nontrivial features, such as *Griffiths singularities in the disordered phase.* Fisher recently examined the critical behavior of this model and derived a number of new results [5].

In this paper, we analyze the *zero-temperature quantum* critical behavior in the opposite limit of infinite dimensionality by examining the quantum Sherrington-Kirkpatrick (SK) model in a uniform transverse field, Γ. To summarize the results for $d=1$ and $d=\infty$: At the zero-temperature spin-glass critical point, Γ_c, the spin autocorrelations decay as a power of $\ln t$ and as t^{-2}, respectively. For $d=1$ both the nonlinear and *linear* susceptibilities diverge *due to Griffiths singularities in portions of the disordered* phase, well away from the critical point [5]. For $d=\infty$, on the other hand, there are no Griffiths singularities, the linear susceptibility always remains finite, and the nonlinear susceptibility diverges *as* Γ_c *is approached from the paramagnetic phase,* with critical exponent $\gamma=\frac{1}{2}$, with a multiplicative logarithmic correction. How the critical behavior varies with dimensionality between these two limits remains an interesting and open question.

Our Hamiltonian,

$$\overline{\mathcal{H}}=-\Gamma\sum_i S_i^z-\sum_{i,j}J_{ij}S_i^xS_j^x\,, \tag{1}$$

reduces to the SK Hamiltonian [6], for $\Gamma=0$. In the second term of (1), the sum is over *all* pairs of spins. The couplings J_{ij} are assumed to have a Gaussian distribution, with mean zero and variance J^2/N, where N is the number of spins. For $N\to\infty$, the model corresponds to (i) the limit of infinite-range interactions, or (ii) the limit of infinite-dimensional space when one considers only one "hyperplaquette" of a close-packed lattice. The components of the spin-$\frac{1}{2}$ spins $\mathbf{S}$ obey the usual commutation relations: $\mathbf{S}_i\times\mathbf{S}_j=i\delta_{ij}\mathbf{S}_i$.

As in the one-dimensional case, the phase diagram of this model has been well delineated, although here no exact solution has been found for finite, nonzero Γ. At zero transverse field the transition temperature is $T_c(\Gamma=0)=J/4$ for spin $\frac{1}{2}$. For sufficiently high temperature, and/or sufficiently large Γ, thermal and/or quantum fluctuations destroy the spin-glass (SG) order, yielding a paramagnet [7]. For low T and small Γ one finds a SG ordered phase, apparently with broken replica symmetry [8]. *Monte Carlo calculation, numerical spin summation [8], and perturbation expansion [9] in* $(1/\Gamma)$ have determined the phase boundary to some precision. As in the classical model, the *infinite-range interactions* apparently wipe out the Griffiths singularities.

Bray and Moore [2] introduced the method by which models of this form have most often been studied. They observed that the average over realizations of the random couplings, J_{ij}, may be performed by means of replicas (or, in the *disordered* phase, within a weak-coupling expansion in J_{ij}), yielding a four-spin interaction. This four-spin interaction they then decouple by means of a Hubbard-Stratonovich transformation, into a form involving an interaction that is nonlocal in imaginary time, τ. In the process, distinct site indices are also decoupled, and the spatial degrees of freedom are completely eliminated. Finally, the number of sites N is taken to infinity, yielding a saddle-point condition on this interaction. These manipulations have been reproduced often enough in the literature [7], so we shall not display them here. Rather, we simply give the Hamiltonian at zero temperature in the form obtained by Bray and Moore:

$$\mathcal{H} = -\frac{1}{2}\int\int_{-\infty}^{\infty} d\tau\, d\tau' J^2 R(\tau-\tau') S^x(\tau) S^x(\tau') + \int_{-\infty}^{\infty} d\tau\, \Gamma S^z(\tau) . \tag{2}$$

Here we consider only the paramagnetic phase and the critical point, where the saddle point is replica symmetric. The saddle-point condition on the nonlocal interaction $R(\tau-\tau')$ is that it is equal to the correlation function $D(\tau-\tau')$:

$$R(\tau-\tau') = D(\tau-\tau') \equiv \langle T S^x(\tau) S^x(\tau')\rangle . \tag{3}$$

The angular brackets denote an average with respect to $\mathcal{H}$, and T indicates time ordering in (3).

It is with the form (2) and (3) that most earlier calculations have begun. By means of the Trotter-Suzuki formula [10], these equations may be recast as a *classical* one-dimensional Ising model with long-range interactions. This classical model may then be studied numerically, by exact spin-summation or Monte Carlo techniques [8]. Most *analytical* work has involved the "static approximation": R is taken to have no time dependence [8]. While this approximation is appropriate for small Γ, it is not valid for $T=0$ and $\Gamma \geq \Gamma_c$, where we anticipate that $R(\tau)$ decays to zero for $\tau \to \infty$. One exception to this body of work is the perturbative and Padé analysis of Yamamoto and Ishii [9], who examined the behavior of the linear and nonlinear susceptibilities as the SG transition is approached from the paramagnetic phase at $T=0$; however, they did not examine the time dependence of the correlations.

Here, we calculate the zero-temperature critical behavior of the correlation function $D(\tau)$, which by (3) coincides with the interaction, $R(\tau)$. Our argument is nonperturbative, and applies directly to the above quantum SK model; we conjecture that the same reasoning (and critical exponents) applies generally to analogous infinite-range quantum vector models. We also introduce a perturbative approximation scheme which gives us the correct critical behavior near Γ_c, and yields, order for order, a value for Γ_c competitive with that yielded by the Padé analysis [9].

In what follows we set J equal to 1 in the Hamiltonian (2). We shall first expand the correlation function of (2), $D(\tau-\tau')$, perturbatively in R about the disordered limit, $R=0$, without imposing the self-consistency condition (3). For $R=0$, we have simply

$$D^0(\tau-\tau') = \tfrac{1}{4}\exp\{-\Gamma|\tau-\tau'|\} . \tag{4}$$

It is convenient for perturbation theory to recast the spins in terms of bilinears in the fermion operators $c_\uparrow, c_\downarrow$. That is, we write [11] $S^\mu(\tau) = c_i^\dagger(\tau) S^\mu_{ij} c_j(\tau)$, where the i,j are summed over $\uparrow,\downarrow$. This formulation allows us to carry out the usual quantum linked-cluster expansion with $\mathcal{H}$. The fermion formulation requires in general a normalization factor *for each distinct spin* in a given term in the perturbation expansion, to correct for the unphysical states in the fermion trace. Our problem *involves exactly one spin*, so in general this normalization would only entail overall multiplication by a single factor. *At zero temperature, in the presence of a gap*, e.g., the transverse field Γ, this factor is unity. Note that D now involves four fermion operators, and takes the form of a polarizability. In this fermion representation, one readily calculates the unperturbed *fermion* propagators:

$$G_\uparrow^0(\omega) = \frac{1/4}{\Gamma/2 - i\omega}, \quad G_\downarrow^{(0)}(\omega) = -\frac{1/4}{\Gamma/2 + i\omega} ; \tag{5}$$

from which the unperturbed S^x propagator immediately follows:

$$D^0(\omega) = \frac{\Gamma}{2(\Gamma^2+\omega^2)} . \tag{6}$$

Transforming to frequency space, and expanding the correlation function $D(\omega)$ within the interaction picture, we find that couplings with the z component of spin make no contribution to $D(\omega)$. We may now express the four-fermion correlation function in terms of the *proper* (irreducible) polarizability [12], $\Pi^*(\omega)$. In particular, we may take advantage of the Ising character of the interaction to write the S^x correlations as [13]

$$D(\omega) = \tilde{\Pi}^*(\omega)/[1 - R(\omega)\tilde{\Pi}^*(\omega)] , \tag{7}$$

where $\tilde{\Pi}^* = 2\,\mathrm{Re}(\Pi^*)$. Imposing the self-consistency condition, $R(\omega) = D(\omega)$ results in a quadratic equation for $D(\omega)$. This equation, as usual, has two solutions, but only the physical one,

$$2D(\omega) = 1/\tilde{\Pi}^*(\omega) - \{[1/\tilde{\Pi}^*(\omega)]^2 - 4\}^{1/2} , \tag{8}$$

behaves properly in the high-frequency limit, $\omega \gg \Gamma$, where $D \approx \tilde{\Pi}^* \sim \omega^{-2}$.

We now claim that general considerations on the form of Π^* (and therefore of $\tilde{\Pi}^*$) are sufficient to establish the low-frequency behavior of $R(\omega)$ at and near the critical point, Γ_c. The uniform linear susceptibilities at the SG transition are *finite*, so we expect *no divergences* in any contribution to Π^*. Observe that, since Π^* denotes the *proper* polarizability, every term in Π^* that depends on ω involves *at least* one frequency integration over $R(\omega)$. In fact, within Π^*, R only occurs in *convolution* with either the Lorentzian form of $D^0(\omega)$, or with some function that has been previously smoothed by convolution with a Lorentzian. It follows that Π^* will be an *analytic* function of ω, even at the critical point when $R(\omega)$ has nonanalyticities at $\omega=0$. With the reasonable assumption that at $\Gamma=\Gamma_c$, the critical R has the small-frequency form

$$R(\omega)=a-b|\omega|^{\zeta}+\cdots,\quad \zeta<2, \tag{9}$$

we immediately conclude that $\tilde{\Pi}^*$ has for its leading contributions in ω the form $c+dw^2$; *no smaller power of ω can appear.* Neglecting, *for the moment,* the question of amplitudes and signs of the other constant terms and coefficients, to satisfy (8) we require $c=\frac{1}{2}$ and $\zeta=1$, yielding a $1/\tau^2$ dependence for the critical $D(\tau)=R(\tau)$ at large τ.

We may also obtain the critical behavior for $\Gamma\to\Gamma_c$ by appealing to the analytic form of $\tilde{\Pi}^*(\omega)$. We expand in ω, defining non-negative Γ-dependent coefficients A and Δ via

$$1/\tilde{\Pi}^*(\omega)=2+A^2(\Delta^2+\omega^2)+O(\omega^4). \tag{10}$$

The expected behavior at $\Gamma=\Gamma_c$ dictates that A remains nonzero for $\Gamma\to\Gamma_c$, while Δ vanishes. The analyticity of $\tilde{\Pi}^*$ eliminates the possibility of divergences in the coefficients of powers of ω, as $\Delta\to 0$. Substitution in (8) gives

$$D(\omega)=1-A(\Delta^2+\omega^2)^{1/2}+A^2(\Delta^2+\omega^2)/2+O(\omega^3,\Delta^3). \tag{11}$$

Because we are working with a spin-$\frac{1}{2}$ model, the spin autocorrelation function at zero time, and thus the integral over all frequencies of (11), is subject to the constraint

$$(1/2\pi)\int_{-\infty}^{\infty}d\omega\, D(\omega)=1/4. \tag{12}$$

This constraint determines how Δ vanishes as $\Gamma\to\Gamma_c$. If we consider the dependence of the integral in (12) on Δ, the strongest nonanalyticity in Δ is readily seen to arise from the radical in (11): its contribution to the integral varies for Δ near zero as

$$\frac{1}{2\pi}\int_{-\Gamma}^{\Gamma}d\omega\{(\Delta^2+\omega^2)^{1/2}-|\omega|\}\approx\tfrac{1}{2}\Delta^2\ln(\Gamma/\Delta). \tag{13}$$

If we make the assumption that the leading nonanalytic dependence of $D(\omega)$ on $\Delta\Gamma\equiv\Gamma-\Gamma_c$ may be subsumed in Δ, we conclude that the Δ dependence given by (13) must be canceled by analytic terms higher order in ω and $\delta\Gamma$ in order to maintain the constraint (12). Consequently, as $\Gamma\to\Gamma_c$, we find $\Delta^2|\ln\Delta|\sim\delta\Gamma$: the gap, Δ, vanishes logarithmically faster than $\sqrt{\delta\Gamma}$. Substituting the form for the linear susceptibility, $\chi_0=D(\omega=0)$, obtained from (11), into the expression for the bulk nonlinear susceptibility [9], χ_2^B, we infer

$$\chi_2^B\sim\frac{1}{1-\chi_0^2}\sim\frac{1}{\Delta}\sim\left(\frac{|\ln\delta\Gamma|}{\delta\Gamma}\right)^{1/2}. \tag{14}$$

Thus the critical exponent γ for the nonlinear susceptibility is $\frac{1}{2}$, and there is a multiplicative logarithmic correction to the usual power law. This expectation is supported by the Padé analysis [9], which estimated $\gamma\cong 0.564$; the logarithmic correction is difficult to distinguish from a small power in a numerical calculation.

It remains for us to examine the constants and coefficients in (8) and (10). Evidently, the vanishing at $\omega=0$ of the expression under the square root in (8) determines Γ_c. Since the interactions in (2) are purely ferromagnetic, we expect $R(\omega)$ and $\tilde{\Pi}^*(\omega)$ to be monotonic in $|\omega|$. The critical singularities we have discussed above rely on the nonvanishing of A; were A to vanish at Γ_c, both the leading critical contributions to $D(\omega)$ and to the scaling of the susceptibility near Γ_c could be analytic in character. In contrast to our nonperturbative argument for the power-law decay of $D(\tau)$ at Γ_c, we are only able to compute *amplitudes* within perturbation theory.

In the following, we shall approximate D using (8), calculating Π^* to zeroth, and then first, order in R. To both orders, we find a critical value of Γ_c within a few percent of the value computed via a Padé analysis by Yamamoto and Ishii [9]. This coincidence of values suggests that our approximations yield quantitative information about amplitudes.

While a computation to all orders in R using (8) would satisfy the constraint (12) exactly, since our fermion representation of the spins satisfies the exclusion principle, *approximations* to Π^* do not necessarily maintain that constraint. To correct any violation of the constraint on $D(\tau=0)$, we may subtract the offending δ function from $R(\tau=0)$. Note that since $R(\tau=0)$ multiplies a c-number, this subtraction does not change any correlations, it represents merely a shift in the zero of energy. Thus our self-consistency condition (3) becomes

$$D(\tau)=R(\tau)-\lambda\delta(\tau), \tag{15}$$

or equivalently in frequency space

$$D(\omega)=R(\omega)-\lambda, \tag{16}$$

where D and R are to be determined by (7), and λ is to be determined self-consistently by the condition (12) that $D(\tau=0)=\frac{1}{4}$.

Calculating $\tilde{\Pi}^*$ to *zeroth* order in R and substituting in (7), we obtain our zeroth-order approximation for Γ_c and the correlations at Γ_c:

$$D(\omega)=1+\omega^2/\Gamma_c-\omega(2/\Gamma_c+\omega^2/\Gamma_c^2)^{1/2}, \tag{17}$$

where

$$\Gamma_c=1+\lambda_c/2=9\pi^2/128. \tag{18}$$

This value of $\Gamma_c \cong 0.694$ is to be compared to the value obtained from the Padé treatment [9] referred to earlier, 0.750. We have also approximated Γ_c by calculating $\tilde{\Pi}^*$ to *first* order in R; solving the ensuing integral equation numerically, we obtain $\Gamma_c = 0.731 \pm 0.005$. At the critical point the coefficient A in (11) is $A_c \cong 1.70$ in the zeroth-order approximation, and $A_c \cong 1.27$ at the first order. We have also evaluated $D(\omega)$ at the critical point, to both zeroth and first orders. We find that the functions differ by at most 2%. These considerations support the validity of our approximations and thus the above analysis of the critical behavior.

We conclude our analysis with a discussion of the behavior near the zero-temperature critical point at low, but nonzero temperature, T. We again take $D(\omega)$ of the form (11), although now ω only takes on the discrete values $\omega_n \equiv 2\pi T n$. As before, the constraint (12), which is now a sum, entails that terms analytic in T and $\delta\Gamma$ cancel against Δ-containing contributions to the sum.

For $T \ll \Delta$, the finite-T correlations, after the frequency integrals are replaced with sums, are of order $\exp(-\{\Delta/T\})$. In this regime, Δ actually represents a *gap*, and quantum mechanics dominates the critical behavior.

For $T \gg \Delta$, the frequency sum has leading Δ-dependent contributions of the form $A\Delta T$ from the $n=0$ term, and $A\Delta^2|\ln T|$ from the sum over nonzero n. There is a Δ-independent finite-T correction varying as T^2. Thus for $T \gg \Delta$, near the zero-temperature critical point we expect

$$A\Delta\{T + \Delta|\ln T|\} \approx aT^2 + b\{\Gamma - \Gamma_c(T=0)\}\,, \tag{19}$$

where we expect the nonuniversal coefficients a and b to be positive. At the finite-temperature phase boundary, Δ vanishes, so we have

$$\Gamma_c(0) - \Gamma_c(T) \approx aT^2/b\,. \tag{20}$$

Near the phase boundary is a *classical* critical regime $\Delta \ll T/|\ln T|$ where

$$\Delta \approx \frac{b\{\Gamma - \Gamma_c(T)\}}{AT}\,. \tag{21}$$

There is also a *crossover* regime $T/|\ln T| \ll \Delta \ll T$, where

$$\Delta^2 \approx \frac{b\{\Gamma - \Gamma_c(T)\}}{A|\ln T|}\,. \tag{22}$$

This discussion completes our characterization of the phase transition and the disordered phase in the vicinity of the zero-temperature critical point.

We close by remarking that an equation closely resembling (8) has been derived earlier [14] by means of a quantum analog of Sompolinsky's dynamical formalism [15]; however, its consequences were examined only within the static approximation [16]. As this paper was being finished, we received a preprint by Ye, S. Sachdev, and N. Read, who obtain the quantum critical behavior for an infinite-range SG of M-component rotors in the large M limit; their results coincide with what we find here for the Ising case.

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