Mean Field Theory of a Quantum Heisenberg Spin Glass

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A full mean-field solution of a quantum Heisenberg spin-glass model is presented in a large-N limit. A spin-glass transition is found for all values of the spin S. The quantum critical regime associated with the quantum transition at $S = 0$ and the various regimes in the spin-glass phase at high spin are analyzed. The specific heat is shown to vanish linearly with temperature. In the spin-glass phase, intriguing connections between the equilibrium properties of the quantum problem and the out-of-equilibrium dynamics of classical models are pointed out.

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The interplay between quantum effects and disorder in spin glasses have been a subject of great recent interest [1]. On the experimental side, the strength of quantum fluctuations can be continuously tuned by varying, e.g., an applied transverse magnetic field [2]. Progress on the theoretical side has followed two different routes. From the higher dimensional end, mean-field solutions and effective Landau theories have been obtained [3,4] for quantum Ising and rotor spin glasses, with a special focus on the vicinity of the quantum-critical point where the glass transition temperature is driven to zero. In low dimensions [5–7], it has been shown that the low-T physics is controlled by rare events (Griffiths-McCoy effects) at strong disorder fixed points.

However, no established mean-field theory of the experimentally important case of quantum Heisenberg spin glasses, with full SU(2) symmetry, is yet available. Unlike the rotor/Ising models above, each site has nontrivial Berry phases which impose the spin commutation relations, and this is expected to place these models in a different universality class [8]. Bray and Moore [9] pioneered the study of a model of Heisenberg spins on a fully connected (Sherrington-Kirkpatrick) lattice of $\mathcal{N}$ sites. In this Letter, we report a full solution of this model, both in the paramagnetic and the glassy phase, when the spin symmetry group is extended from SU(2) to SU(N) and the large-N limit is taken. The Hamiltonian is

$$H = \frac{1}{\sqrt{\mathcal{N} N}} \sum_{i<j} J_{ij} \vec{S}_i \cdot \vec{S}_j \,, \tag{1}$$

where the J_{ij} are independent, quenched random variables with distribution: $P(J_{ij}) \propto e^{-J_{ij}^2/(2J^2)}$. In an imaginary time path-integral formalism, the model is mapped onto a *self-consistent single site* problem with the action [8,9]

$$S_{\rm eff} = S_B + \frac{J^2}{2N} \int_0^\beta d\tau\, d\tau'\, Q^{ab}(\tau - \tau') \vec{S}^a(\tau) \cdot \vec{S}^b(\tau') \,, \tag{2}$$

with $\beta = 1/k_B T$, and the retarded interaction $Q^{ab}(\tau - \tau')$ obeys the self-consistency condition

$$Q^{ab}(\tau - \tau') = (1/N^2) \langle \vec{S}^a(\tau) \vec{S}^b(\tau') \rangle_{S_{\rm eff}} \,. \tag{3}$$

Here, $a, b = 1, \ldots, n$ denote the replica indices (the limit $n \to 0$ has to be taken later), and S_B is the Berry phase in the spin coherent state path integral. For $N = 2$ the problem remains of considerable difficulty even in this mean-field limit. In [9], as well as in most subsequent work [10], the *static approximation* was used in which the τ dependence of $Q^{ab}(\tau)$ is neglected; this may be appropriate in some regimes but prevents a study of the quantum equilibrium dynamics, in particular, in the quantum-critical regime. This imaginary time dynamics has, however, been studied recently in a Monte Carlo simulation with spin $S = 1/2$ by Grempel and Rozenberg [11], but their study was limited to the paramagnetic phase. In our large-N limit, the problem is exactly solvable and, as explained below, this limit provides a good description of the physics of the $N = 2$ mean-field model, as far as the latter is known. We find that in the paramagnetic phase, at low S (where the quantum fluctuations are the strongest), the quantum-critical regime is a *gapless* quantum paramagnet already studied in [8,12] and radically different from the paramagnet obtained in the classical regime (at large S), in which a local moment behavior persists down to the glass transition. In the spin-glass phase, various regimes are obtained as a function of temperature T. The thermodynamic properties and the dynamical response functions are analyzed below. Most notably, the low-T specific heat is found to have a linear T dependence, a behavior commonly observed experimentally in spin glasses but not often realized in mean-field *classical* models. Furthermore, the equilibrium dynamics of the quantum case reveals intriguing connections with some known features of the out-of equilibrium dynamics of classical glassy models, an observation already made in [13] in a different context.

To handle the large-N limit, we use a Schwinger boson representation of the SU(N) spin operators: $S_{\alpha\beta} = b_\alpha^\dagger b_\beta - S\delta_{\alpha\beta}$, corresponding to fully symmetric representations (one line of NS boxes in the language of Young tableaux) where the number of bosons is constrained by

$\sum_\alpha b_\alpha^\dagger b_\alpha = NS$. In the SU(2) case, S coincides with the usual definition of spin. Fermionic representations can also be considered but they actually do not lead to a spin-glass phase at any temperature in the $N = \infty$ limit [8]. In the large-N limit, the self-consistent single-site problem reduces to a nonlinear integral equation for the replicated boson Green's function: $G^{ab}(\tau) \equiv -\sum_\alpha \langle T b_\alpha^a(\tau) \times b_\alpha^{\dagger b}(0)\rangle / N$ [8]:

$$(G^{-1})^{ab}(i\nu_n) = i\nu_n \delta_{ab} + \lambda^a \delta_{ab} - \Sigma^{ab}(i\nu_n), \quad (4)$$

$$\Sigma^{ab}(\tau) = J^2 \Big(G^{ab}(\tau)\Big)^2 G^{ab}(-\tau), \quad (5)$$

$$G^{aa}(\tau = 0^-) = -S. \quad (6)$$

Here, ν_n are the bosonic Matsubara frequencies, and G^{-1} stands for the inverse in replica space. The (disorder-averaged) local spin correlation function is related to $G^{ab}(\tau)$ by $\chi_{\rm loc}(\tau) \equiv \overline{\langle \vec{S}_i(0) \cdot \vec{S}_i(\tau)\rangle} = G^{aa}(\tau) G^{aa}(-\tau)$. The resulting phase diagram, obtained by both analytical and numerical studies of these equations, is displayed in Fig. 1, as a function of S and T/J. Spin-glass ordering is found at any value of S. The critical temperature increases as JS^2 at large S (see below) and vanishes in the limit $S \to 0$, as found earlier in [10]. The point $S = 0$, $T = 0$ is the quantum critical point of this model. Several crossovers are found *within* the spin-glass phase, which will be described later.

We first describe the paramagnetic phase and the associated crossovers. In this phase, the Green's function is replica diagonal $G^{ab}(\tau) = G(\tau)\delta_{ab}$ and thus Eqs. (4)–(6) reduce to a single nonlinear integral equation. We emphasize that, as in any mean-field theory, paramagnetic solutions of the mean-field equations can be found even below the critical T where an instability to ordering occurs. At high T, we have nearly free spins with an almost constant correlation function $\chi_{\rm loc}(\tau) \simeq S(S+1)$ and a Curie local susceptibility $\chi_{\rm loc} \equiv \int_0^\beta \chi_{\rm loc}(\tau)\, d\tau \simeq S(S+1)/T$.

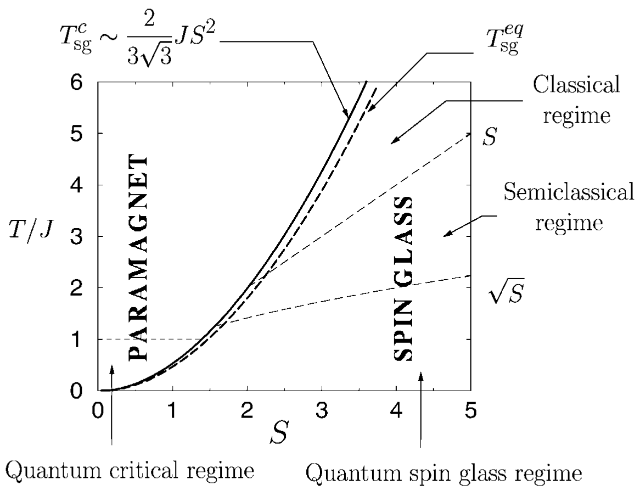

FIG. 1. Mean-field phase diagram and crossovers of the large-N quantum Heisenberg spin glass (the various regimes are discussed in the text).

For large values of S, these solutions smoothly evolve, as T is reduced, into solutions which still behave locally as local moments, but with a Curie constant reduced by quantum fluctuations: $\chi_{\rm loc} \simeq S^2/T$. This partial quenching occurs at a temperature of order JS^2 at large S, of the same order but *smaller* than the glass transition temperature. These solutions actually have unphysical low-T properties, such as a divergent internal energy $U \simeq -J^2 S^4/2T$ and a negative entropy ($\propto -J^2 S^4/4T^2$). These features are well known in classical mean-field models and simply signal the tendency to spin-glass ordering. At smaller values of S (Fig. 1), a crossover to a different kind of paramagnetic solution is found below $T \simeq J$, where we enter the quantum-critical regime. In this gapless quantum paramagnet (spin liquid), investigated previously in [8,12], the local response displays a scaling form for $\omega, T \ll J$, $J\chi''_{\rm loc}(\omega) \propto \tanh(\omega/2T)$, and the local susceptibility diverges only logarithmically $J\chi_{\rm loc} \propto \ln(J/T)$. In contrast to the local-moment solutions, this paramagnet has finite residual low-temperature entropy [14], so that the quenching of the entropy as T is decreased takes place much more gradually at low S, when quantum fluctuations are strong, than at large S in the classical regime. It can be shown analytically [14] that these solutions of the mean-field equations exist down to $T = 0$ only for very low values of S, smaller than $S_c \simeq 0.05$. For larger spins, a local-moment-like solution is retrieved as T is lowered below a temperature of order JS^2 (again below the actual glass transition). However, the spin-liquid solutions are the relevant ones in the quantum-critical regime *at finite temperature* $JS^2 < T < J$ for an extended range of spin values which extend up to $S \simeq 1$. The detailed analysis of the coexistence between these two kinds of paramagnetic solutions at low S is rather intricate and will be presented elsewhere [14].

In the quantum Monte Carlo results of [11] for the paramagnetic phase of the $S = 1/2$, SU(2) model, the same reduction of the Curie constant from $S(S+1)$ to S^2 was observed. Furthermore, the relaxation function $\chi''(\omega)/\omega$ evolves from a single peak of width JS centered at $\omega = 0$ to a three peak structure in the low-T local moment regime. The central peak of weight S^2 corresponds to the residual local moment while two side peaks at an energy scale J^2S^3/T correspond to transverse relaxation [11]. All these features are captured by our solution in the large-N limit, the only qualitative difference being that no thermal broadening of the central peak is found in this limit. Furthermore [15], numerical results not reported in [11] reveal that, in a limited intermediate T range of the SU(2) $S = 1/2$ model, spin liquid solutions similar to those found here in the quantum-critical regime are observed. Although a logarithmic regime is not directly visible in the T dependence of the local susceptibility because of this limited range, quantum criticality is directly apparent in a nonmonotonic T dependence of the local spin correlation function $\chi_{\rm loc}(\tau)$.

We now turn to the analysis of the spin-glass phase. We first note that the spin-glass transition is *not* signaled by the divergence of the spin-glass susceptibility (which is actually of order $1/N$) [14,16]. In the ordered phase, the boson Green's function can be parametrized as follows:

$$G_{ab}(\tau) = [\tilde{G}(\tau) - \tilde{g}]\delta_{ab} - g_{ab}(1 - \delta_{ab}), \quad (7)$$

where g_{ab} is a constant $n \times n$ matrix and g_1 a constant, fixed so that $\tilde{G}$ is regular at $T = 0$, i.e., $\tilde{G}(\tau \to \infty) = 0$. The usual spin-glass order parameter [17] is $q_{ab} = g_{ab}^2$. We have searched for replica-symmetric broken solutions with a general Parisi ansatz for g_{ab} and found only *single-step* replica symmetry breaking solutions (as in [10]). The Parisi function $g(x)$ associated with g_{ab} is thus piecewise constant: $g(x) = 0$ for $x < x_c$, $g(x) = g(1) = \sqrt{q_{\mathrm{EA}}} \equiv g$ for $x > x_c$, where q_{EA} is the Edwards-Anderson order parameter; this also implies that $\tilde{g} = g$. For the following discussion, it is convenient to define the parameter $\Theta \equiv -J\tilde{G}(i\nu = 0)/g$. Using standard inversion formulas for a Parisi matrix [18], the full set of mean-field equations read

$$[\tilde{G}(i\nu_n)]^{-1} = i\nu_n - Jg/\Theta - [\tilde{\Sigma}(i\nu_n) - \tilde{\Sigma}(0)], \quad (8)$$

$$\tilde{\Sigma}(\tau) \equiv J^2[\tilde{G}^2(\tau)\tilde{G}(-\tau) - 2g\tilde{G}(\tau)\tilde{G}(-\tau) - g\tilde{G}^2(\tau) + 2g^2\tilde{G}(\tau) + g^2\tilde{G}(-\tau)], \quad (9)$$

$$\tilde{G}(\tau = 0^-) = g - S, \quad (10)$$

$$\beta x_c = (1/\Theta - \Theta)/Jg^2. \quad (11)$$

However, these equations *do not determine* Θ (or equivalently the breakpoint x_c) as also happens in a classical spin-glass model with a single step of replica symmetry breaking: there is a continuous family of solutions parametrized by Θ, which has to be determined by independent considerations. Two possibilities have appeared in previous work: (i) Determine Θ by minimizing the free energy, as a function of Θ, or (ii) impose a vanishing lowest eigenvalue of the fluctuation matrix in the replica space (the "replicon" mode). Criterion (i) is certainly the natural one from the point of view of equilibrium thermodynamics. However, studies of out-of-equilibrium dynamics of classical spin glasses have revealed [19] that these lowest free-energy solutions can never be reached and that the system "freezes" at a dynamical temperature T_{sg}^c, given precisely by the onset of solutions satisfying the replicon criterion (ii). In our quantum problem, both choices give sensible solutions, but with entirely different spectra of *equilibrium* dynamical fluctuations: (i) leads to a *gap* in $\chi''_{\mathrm{loc}}(\omega)$, while (ii) is found to be the *unique* choice leading to a gapless spectrum. A similar observation was made in the work of Giamarchi and Le Doussal [13] in their study of a one-dimensional quantum model with disorder. In the present context, it seems natural to expect local gapless modes in the ordered phase of a quantum spin glass with continuous spin symmetry, and these various considerations lead us to adopt (ii). Diagonalizing the fluctuation matrix in replica space, we verified stability and obtained the lowest eigenvalue $e_1 = 3\beta J^2 g^2(1 - 3\Theta^2)$. The replicon criterion thus leads to $\Theta = 1/\sqrt{3}$. The same value is also selected by imposing that $\tilde{G}$ has a gapless spectral weight. In contrast, criterion (i) leads to $2\ln\Theta + 1/(4\Theta^2) + 1/2 - 3\Theta^2/4 = 0$, or $\Theta \simeq 0.44\ldots$, and a gapped solution, which is also stable because $e_1 > 0$. We also note that the previous computation shows that the replica symmetric solution $\Theta = 1$ is unstable in the spin-glass phase. Moreover, it can be shown that it leads to unphysical negative spectral weight at large S. Hence, a correct description of the low-energy excitations of the quantum model requires replica symmetry breaking at any finite T in the spin-glass phase, although the replica symmetry is restored at $T = 0$ where $x_c = 0$ [from (11)].

Once Θ is determined, a full numerical solution of the above equations can be performed. In particular, the "equilibrium" spin-glass temperature T_{sg}^{eq} obtained from criterion (i) is *lower* than the "dynamical" transition temperature T_{sg}^c obtained from criterion (ii) (see Fig. 1): this is not obvious *a priori,* but is certainly required in our interpretation. Further analytical insight can be obtained in the limit of large S. This limit can actually be taken in two distinct ways, revealing two crossovers within the spin-glass phase displayed in Fig. 1. If we take $S \to \infty$ while keeping T/JS^2 fixed (i.e., staying close to the critical temperature), all nonzero Matsubara frequencies can be neglected (the static approximation is accurate). In this limit, we find, in particular, $T_{\mathrm{sg}}^c \sim 2JS^2/3^{3/2}$. Alternatively, keeping $\bar{T} = T/JS$ and $\bar{\omega} = \omega/JS$ fixed, we access the "semiclassical" regime of the spin-glass phase. In this limit, the Green's function obeys a scaling form $\tilde{G}(\omega, T) = f(\bar{\omega})/(JS)$, where f turns out to be independent of $\bar{T}$ and satisfies

$$f(\bar{\omega})^{-1} = \bar{\omega} - 1/\Theta - 3\Theta - f(\bar{\omega}) - f^*(-\bar{\omega}). \quad (12)$$

Eliminating $f^*(-\bar{\omega})$ leads to a quartic equation for $f(\bar{\omega})$ on which all the above properties can be checked more explicitly. A plot of the (gapless) relaxation function in the

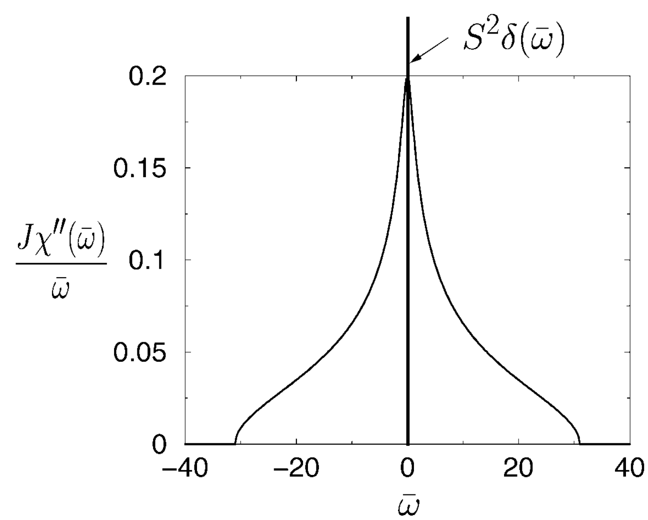

FIG. 2. Relaxation function $\chi''(\omega)/\omega$ in the large-S limit, obtained from (12).

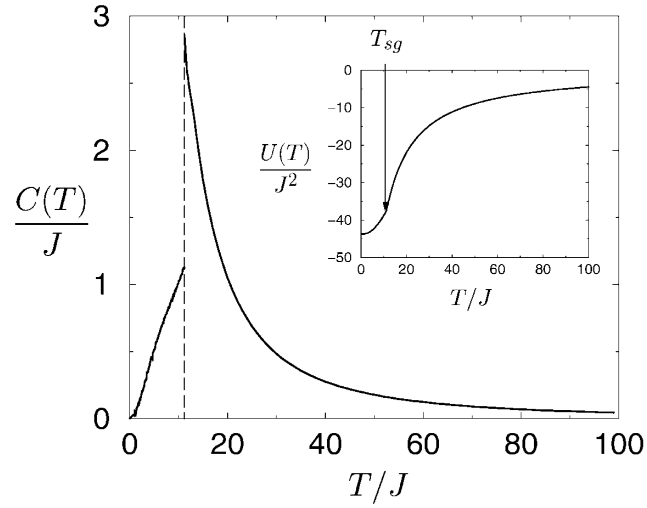

FIG. 3. Specific heat $C(T)$ and internal energy $U(T)$ (inset) vs temperature T, from a numerical solution of Eqs. (8)–(11) for $S = 5$.

spin-glass phase $\chi''(\bar{\omega})/\bar{\omega}$ obtained from (12) is displayed in Fig. 2.

Finally, we briefly describe the thermodynamic properties, focusing on the T dependence of the specific heat. Numerical results for this quantity for intermediate spin are displayed on Fig. 3. They have been obtained from the T derivative of the internal energy $U = -J^2/2 \times \int_0^\beta G_{ab}(\tau)^2 G_{ab}(-\tau)^2 \, d\tau$, where G is a numerical solution of Eqs. (8)–(11). Furthermore, a large-S, low-T expansion of $U(T)$ can be done analytically and leads to [14]: $U(T) = U(0) + aS\bar{T}^4 + b\bar{T}^2 + \ldots$ where a and b are positive numerical coefficients. Hence, in the quantum regime defined by $T < J\sqrt{S}$ (see Fig. 1), the specific heat depends *linearly on temperature*. Moreover, this behavior actually holds numerically for intermediate values of the spin as displayed in Fig. 3.

Despite being formulated over two decades ago [9], a complete understanding of the quantum Heisenberg spin glass at the mean-field level has proven elusive. Here, we have obtained a complete solution in a large-N limit, and presented evidence that global aspects of the phase diagram pertain also to the physical SU($N = 2$) case. We described crossovers in the vicinity of a quantum critical point accessed by varying the spin S, but we can expect that some features and intermediate temperature regimes will survive when it is accessed by varying other parameters in the Hamiltonian, including doping with metallic carriers as in Kondo lattice models [12,20]. We have also described the $T \to 0$ thermodynamics and spectral functions within the spin-glass phase, which is something not previously analyzed in any mean-field quantum spin-glass model: we found a specific heat linear in temperature, and a dynamical susceptibility $\chi''(\omega)/\omega \to$ const as $\omega \to 0$.

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Note added.—It has been recently proven by one of us [21] that the behavior $J\chi''_{\text{loc}}(\omega) \propto$ const found above in the quantum critical regime also holds for SU(2).

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