Mean Field Theory of a Quantum Heisenberg Spin Glass

Antoine Georges\textsuperscript{1}, Olivier Parcollet\textsuperscript{1,2}, and Subir Sachdev\textsuperscript{3}

\textsuperscript{1}CNRS - Laboratoire de Physique Théorique, Ecole Normale Supérieure, 24 Rue Lhomond 75005 Paris FRANCE
\textsuperscript{2}Serin Physics Laboratory, Rutgers University, Piscataway, NJ 08854 USA
\textsuperscript{3}Department of Physics, Yale University, P.O. Box 208120, New Haven, CT 06520-8120, USA

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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.

\begin{equation}
Q^{ab}(\tau - \tau') = \frac{1}{N^2} \langle \hat{S}^a(\tau) \hat{S}^b(\tau') \rangle_{\text{eff}}.
\end{equation}

Here, $a, b = 1, \cdots, n$ 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 \textsuperscript{12}, as well as in most subsequent work, the static approximation was used (see however \textsuperscript{11}), neglecting the $\tau$-dependence of $Q^{ab}(\tau)$: 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 \textsuperscript{13}, 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 \textsuperscript{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 \textsuperscript{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, $S$ co-
The averaged local spin correlation function is related to \( \chi_{\text{loc}} \), which stands for the inverse in replica space. The (disorder-ν) large-N limit of \( \chi_{\text{loc}} \) can be found even below the critical 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 \( U \approx -J^2 S^4 / 2T \) 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 \( T \approx J \), where we enter the quantum critical regime. In this gapless quantum paramagnet (‘spin-liquid’), investigated previously in [8,2], the local response displays a scaling form for \( \omega, T \ll J \), \( J\chi''_{\text{loc}}(\omega) \propto \tanh(\omega / 2T) \), and the local susceptibility diverges only logarithmically \( J\chi_{\text{loc}} \propto \ln(J/T) \). In contrast to the local-moment solutions, this paramagnet has finite residual low-temperature entropy [4], 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 [4] that these solutions of the mean-field equations exist down to \( T = 0 \) only for very low values of \( S \), smaller than \( S_c \approx 0.05 \). 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 \( S \approx 1 \). The detailed analysis of the coexistence between these two kinds of paramagnetic solutions at low \( S \) is rather intricate and will be presented elsewhere [1].

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 \( \chi''(\omega) \approx \omega \) 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 \( J^2 S^3 / T \) 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 [13], numerical results not reported in [11] reveal that in a limited intermediate \( T \) range of the \( SU(2) \) 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 non-monotonic \( T \) dependence of the local spin correlation function \( \chi_{\text{loc}}(\tau) \).

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

$$G_{ab}(\tau) = \left(\tilde{G}(\tau) - \tilde{g}\right) \delta_{ab} - g_{ab}(1 - \delta_{ab})$$  \hspace{1cm} (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-symmetry broken solutions by making a Parisi Ansatz for $g_{ab}$ and found that single-step replica symmetry breaking always applies \[10\]. The Parisi function $g(x)$ associated with $g_{ab}$ is thus piecewise constant: $g(x) = 0$ for $x < x_c$, $g(x) = g(1) = \sqrt{q_{EA}} \equiv \tilde{g}$ 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 $\Theta \equiv -J\tilde{G}(iv = 0)/g$. Using standard inversion formulas for a Parisi matrix \[13\], the full set of mean-field equations read:

$$\left(\tilde{G}(iv_n)\right)^{-1} = iv_n - Jg/\Theta - \left(\tilde{\Sigma}(iv_n) - \tilde{\Sigma}(0)\right)$$  \hspace{1cm} (8)

$$\tilde{\Sigma}(\tau) \equiv J^2 \left(\tilde{G}^2(\tau)\tilde{g}(\tau) - 2g\tilde{G}(\tau)\tilde{g}(\tau) - g\tilde{G}(\tau)\tilde{g}(\tau)\right)$$  \hspace{1cm} (9)

$$\tilde{G}(\tau = 0^-) = g - S$$  \hspace{1cm} (10)

$$\beta x_c = (1/\Theta - \Theta)/Jg^2$$  \hspace{1cm} (11)

However, these equations do not determine $\Theta$ (or equivalently the breakpoint $x_c$) as also happens in classical spin-glass model with a single-step of replica symmetry breaking: there is a continuous family of solutions parametrized by $\Theta$, which has to be determined by independent considerations. Two possibilities have appeared in previous work: (i) Determine $\Theta$ by minimizing the free energy, as a function of $\Theta$, 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 \[18\] 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 $\chi''_{loc}(\omega)$, 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 find the lowest eigenvalue $e_1 = 3\beta J^2 g^2 (1 - 3\Theta^2)$ so that the replicon criterion leads to $\Theta = 1/\sqrt{3}$, independent of $T$; the same value also appears by independently imposing that $\tilde{G}$ has a gapless spectral weight. In contrast, criterion (i) leads to $2\ln(1/(4\Theta^2) + 1/2 - 3\Theta^2) = 0$, or $\Theta \simeq 0.44\ldots$, and a gapped solution. 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 $\Theta$ is determined, a full numerical solution of the above equations can be performed. In particular, the “equilibrium” spin glass temperature $T_{eq}^sg$ obtained from criterion (i) is lower than the “dynamical” transition temperature $T_{sg}^c$ obtained from criterion (ii) (see Fig. 4); 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. 4. If we take $S \to \infty$ while keeping $T/JS^2$ fixed (i.e. staying close to the critical temperature), all non-zero Matsubara frequencies can be neglected (the static approximation is accurate). In this limit, we find in particular $T_{eq}^sg \sim 2JS^2/3^{3/2}$. Alternatively, keeping $T = T/JS$ and $\bar{\omega} = \omega/JS$ fixed, we access the “semi-classical” 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 $T$ and satisfies:

$$f(\bar{\omega})^{-1} = \bar{\omega} - 1/\Theta - 3\Theta - f(\bar{\omega}) - f^*(\bar{\omega})$$  \hspace{1cm} (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 spin-glass phase $\chi''(\omega)/\omega$ obtained from \[12\] is displayed in Fig. 4.

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 $U = -J^2/2 \int_0^1 G_{ab}(\tau)G_{ab}(\tau) - g^2d\tau$, where $G$ is a numerical solution of Eqs.\[8\]-\[10\]. Furthermore, a large-$S$, low-$T$ expansion of $U(T)$ can be done analytically and leads to \[14\]: $U(T) = U(0) + aS^{1/2} + bT^2 + \ldots$ 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.

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

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