Quantum spherical description of an Ising spin glass in a transverse field

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We study the competition between bond randomness and quantum fluctuation in the infinite-range Ising model in the transverse field Δ relevant for a number of pseudospin and magnetic quantum spin-glass systems. By introducing a mapping of the quantum Hamiltonian of the model onto a soft-spin action we consider it truncated version in a form of the solvable quantized spherical model. The resulting critical phase boundary $T_{\rm crit}(\Delta)$ is in considerable agreement with the numerical estimates based on the Trotter-Suzuki and Monte Carlo methods. The equation of state for the system is also given. [S0163-1829(97)05209-0]

The role of quantum fluctuations in spin glasses (SG) remains a long standing theoretical problem (see, Ref. 1, and references therein). One of the simplest for the theoretical study but physically relevant system— the Ising spin glass in a transverse field has attracted renewed interest, especially in relation to the quantum analogue of the Sherrington-Kirkpatrick model[2] (see, e.g., Ref. 3). On the experimental side, there has been also a renewed interest in systems which display the SG transition the vicinity of $T=0$ induced by an external parameter. These include the so-called proton glasses,[4–6] being a random mixture of ferroelectric and antiferroelectric materials such as $Rb_{1-x}(NH_4)_xH_2PO_4$, where the proton tunneling in the glass state can be represented by transverse field in the pseudospin Ising model. In the domain of magnetic systems the long-ranged dipolar insulating Ising spin glass $LiHo_{0.167}Y_{0.833}F_4$ has been studied in the presence of a transverse magnetic field Δ, from which a phase diagram $T_{\rm crit}(\Delta)$ was determined.[7,8]

The system in question displaying the interplay between randomness and quantum fluctuations is described by the following model:

$$H=-\sum_{i<j} J_{ij}\sigma_{iz}\sigma_{jz}-\Delta\sum_{i} \sigma_{ix}. \tag{1}$$

Here σ_x,σ_z are the x,z components of the Pauli spin operators, with the Pauli operators on different sites commuting with each other. For simplicity we consider the interactions J_{ij} as being infinite-range and Gaussian-random distributed variables with zero mean and the variance $J/\sqrt{N}$ (which ensures a sensible thermodynamic limit $N\to\infty$).

Within a pseudospin description of hydrogen-bonded proton glass systems, the proton position in the two potential minima is represented by Ising states, $\sigma_z=\pm1$, and the tunneling between the minima by a transverse field term $\Delta\sigma_x$, where Δ is the tunneling frequency.[9] Each site, therefore, has an Ising degree of freedom while $\Delta\sigma_{ix}$ is the kinetic energy term and induces on-site flips of the Ising spins due to Δ. Thus the transverse field is acting against the SG phase eventually destroying the glassy order even at $T=0$.

A systematic analytic study of the quantum spin glasses is complicated by two factors: (1) the problem has a dynamical nature from the outset and cannot be simplified to calculation of static quantities even while evaluating statistical mechanical averages; (2) quenched disorder and associated very complicated energy landscape resulting in a huge number of local minima of free energy as in the case of the classical spin glasses. Usually, an approximate analytically tractable solution to the problem can be obtained by replacing the dynamic self-interaction by an appropriate time average. In the context of the Matsubara ''imaginary time'' and replica approach this method is referred to as the static approximation.[10] While conceptually simple, this approximation offers a rather crude description due to effective suppression of quantum fluctuations. An essential improvement can be obtained by finding a way of systematic parameterization of quantum correlations.[11] It would be desirable to go beyond static theory but there is no hope in solving any realistic quantum SG exactly. It may therefore be useful to study quantum spherical models[12] of disordered systems, where the analysis can be pushed further.

To this end we introduce in the present paper a mapping of the quantum Hamiltonian (1) onto a soft-spin action containing quantum correlations of arbitrary order considering furthermore its truncated version in a form of the solvable quantized spherical model.

The model (1) should be contrasted with another system, namely, the SG of quantum rotors solved in the large-M vector limit.[13,14] There, the quantum dynamics was associated with a finite moment of inertia of rotors. Although it has been argued that it is natural to consider the transverse-field Ising model as simply the $M=1$ case of quantum rotors[15] (as a formal limiting case, of course, since $M\geqslant 2$ for rotors) there are important differences in symmetries between the Hamiltonian (1): O(M) rotational symmetry in the rotor model vs discrete $\mathcal{Z}_2$ symmetry in the transverse Ising spin glass. As we shall see our detailed analysis shows that there is no one-to-one mapping between quantum rotor model and quantized spherical model obtained for the transverse Ising SG and, consequently, details of thermodynamic behavior will differ in both cases.

It is convenient to express the partition function $Z = \mathrm{Tr}\exp(-\beta H)$ of the model (1) in the interaction representation as

$$Z = \mathrm{Tr} e^{-\beta H_0} T_\tau \exp\left[-\int_0^\beta d\tau \sum_{i<j} J_{ij}\sigma_{iz}(\tau)\sigma_{jz}(\tau)\right] \quad (2)$$

with the interaction picture Hamiltonian H-H_0 and the ''free'' part

$$H_0 = -\Delta \sum_i \sigma_{ix} \quad (3)$$

so that the statistical average can be taken in the ensemble given by H_0. Here, $\beta = 1/k_B T$ with T being the temperature, T_τ is the Matsubara ''imaginary time'' ordering operator allowing us to treat the time dependent operators $\sigma_{iz}(\tau) = e^{-\tau H_0}\sigma_{iz} e^{\tau H_0}$ as c numbers within the time-ordered exponential (2). This turns out to be very convenient because it enables us to handle the objects $\sigma_{iz}(\tau)$ as bosonic fields. We introduce new continuous fields $m_i(\tau)$ using the identity

$$\delta[\xi - \xi'] = \int \mathcal{D}\left(\frac{\zeta}{2\pi i}\right) e^{-(\xi-\xi')\zeta}, \quad (4)$$

where $\xi\zeta \equiv \int_0^\beta d\tau \xi(\tau)\zeta(\tau)$. In spite of the singular character of $\delta[\xi - \xi']$ it plays exactly the same role for functionals as the conventional Dirac delta function in calculations involving δ-function. Using the above relation and the c-number property of $\sigma_z(\tau)$ (under the ''imaginary'' time ordering operator T_τ) we may rewrite the statistical sum (2) as follows

$$Z = \int \prod_i Dm_i \, \mathrm{Tr} e^{-\beta H_0} \prod_i T_\tau \delta[m_i(\tau) - \sigma_{iz}(\tau)] \delta\left[\sum_i m_i^2(\tau) - N\right] \times \exp\left[-\int_0^\beta d\tau \sum_{i<j} J_{ij} m_i(\tau) m_j(\tau)\right]. \quad (5)$$

The technique employed in deriving of Eq. (5) can be considered as a generalized version of widely used the so-called Hubbard-Stratonovich formula. This becomes apparent inferring the integral representation of the δ function [see, Eq. (4)]: we obtain similar integral expression involving exponential with auxiliary field coupled to $\sigma_z(\tau)$.

According to the construction of the statistical sum (5) the continuous field variables $m_i(\tau)$ are allowed to take all values $-\infty < m_i(\tau) < \infty$. However, the original pseudospin variables obey $\sigma_{iz}^2(\tau) = 1$ at each site. While an exact computation of Z in terms of the functional integral over $m_i(\tau)$ should conform to this restriction an approximation in evaluation of Z does not necessarily maintain that constraint. Therefore, to enforce the constraint we included the term $\delta[\Sigma_i m_i^2(\tau) - N]$ in Eq. (5). Note, that we have also relaxed the ''strong'' constraint $m_i^2(\tau) = 1$ (all i) and imposed instead the ''weak'' one: $\Sigma_i m_i^2(\tau) = N$ which allow us to make contact with solvable ''mean spherical'' model.

Utilizing Fourier representation (4) of the δ functional we have

$$Z = \int Dz \prod_i Dm_i D\mu_i \exp\left[-\int_0^\beta d\tau \sum_{ij} J_{ij} m_i(\tau) m_i(\tau) + \int_0^\beta d\tau \sum_i (m_i^2(\tau) - N) z(\tau)\right] \times \exp\left[-\int_0^\beta d\tau \sum_i m_i(\tau)\mu_i(\tau) + W_i^{(0)}[\mu]\right]. \quad (6)$$

Here, $\mu_i(\tau)$ and $z(\tau)$ are variables coupled to $\sigma_{iz}(\tau)$ and $m_i^2(\tau)$, respectively (the Lagrange multipliers) while $W_i^{(0)}[\mu] = \ln Z_i^{(0)}[\mu]$ with

$$Z_i^{(0)}[\mu] = \mathrm{Tr}_\sigma e^{-\beta H_0} T_\tau \exp\left[\int_0^\beta d\tau \sigma_{iz}(\tau)\mu_i(\tau)\right] \quad (7)$$

being the generating functional of the complete pseudospin Green's functions for the noninteracting system in the Matsubara formalism. It is well known that related functional $W_i^{(0)}[\mu]$ is just the generating functional for the connected Green's functions $K_{0ni}(\tau_1, \ldots, \tau_\ell)$ (cumulants) and

$$W_i^{(0)}[\mu] = \sum_{s=1}^\infty \frac{1}{s!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_\ell K_{0si}(\tau_1, \ldots, \tau_s) \times \mu_i(\tau_1) \cdots \mu_i(\tau_s), \quad (8)$$

where $K_{0si}(\tau_1, \ldots, \tau_s) = \langle T_\tau \sigma_{iz}(\tau_1) \cdots \sigma_{iz}(\tau_s)\rangle_0^{\mathrm{cum}}$. Here, for given operators $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ the cumulant averages are defined as $\langle \mathcal{AB}\rangle_0^{\mathrm{cum}} = \langle \mathcal{AB}\rangle_0 - \langle \mathcal{A}\rangle_0 \langle \mathcal{B}\rangle_0$, $\langle \mathcal{ABC}\rangle_0^c = \langle \mathcal{ABC}\rangle_0 - \langle \mathcal{A}\rangle_0\langle \mathcal{BC}\rangle_0 - \langle \mathcal{B}\rangle_0\langle \mathcal{AC}\rangle_0 - \langle \mathcal{C}\rangle_0\langle \mathcal{AB}\rangle_0 + 2\langle \mathcal{A}\rangle_0\langle \mathcal{B}\rangle_0\langle \mathcal{C}\rangle_0$, $\ldots$, etc., where $\langle \cdots \rangle_0 = \mathrm{Tr} \cdots \exp(-\beta H_0)/\mathrm{Tr}\exp(-\beta H_0)$.

Since the generic spherical model consists of the Gaussian part in fluctuating constrained fields we include only terms in the exponential of Eq. (6) which are quadratic in the fluctuating ''spin density'' $m_i(\tau)$. Expanding $W_i^{(0)}[\mu]$ to the second order in μ_i and integrating out the μ_i fields we obtain the statistical sum of the quantum version of the spherical (QSP) model

$$Z_{\mathrm{QSP}} = \int \prod_i \mathcal{D}m_i \int \mathcal{D}\left[\frac{z}{2\pi}\right] e^{-S_{\mathrm{QSP}}[m,z]}, \quad (9)$$

where the quadratic action reads

$$S_{\mathrm{QSP}}[m,z] = \frac{1}{2}\int_0^\beta d\tau d\tau' \left\{ \sum_{ij} [(J_{ij} - 2z(\tau)\delta_{ij})\delta(\tau-\tau') + \delta_{ij}K_{02}^{-1}(\tau-\tau')] m_i(\tau) m_j(\tau') + Nz(\tau)\delta(\tau-\tau')\right\}, \quad (10)$$

where $K_{02}^{-1}(\tau-\tau')$ is the inverse function of $K_{02}(\tau-\tau')$. Furthermore,

$$K_{02}(\tau-\tau') = \frac{2}{Z_0}\{\cosh[\beta\Delta - 2\Delta(\tau-\tau')]\Theta(\tau-\tau') + \cosh[\beta\Delta + 2\Delta(\tau-\tau')]\Theta(\tau'-\tau)\}, \quad (11)$$

where $Z_0=2\cosh(\beta\Delta)$ and $\Theta(x)$ is the step function. Due to the presence of the Lagrange multipliers z [the action (10) is augmented by the term $z(\tau)m_i^2(\tau)$ the integration takes place over all finite energy configurations of $m_i(\tau)$ variables]. Because the model is now effectively unconstrained and quadratic all the quantities can be computed readily. In the thermodynamic limit $N\to\infty$ the saddle point method gives the condition of constraint in a form of an implicit equation for the Lagrange multiplier $z(T,\Delta)$

$$1=\frac{1}{N}\sum_i \overline{\langle m_i(\tau)m_i(\tau+0)\rangle}_{\mathrm{QSP}}, \tag{12}$$

where the bar denotes averaging over the quenched disorder and

$$\langle\cdots\rangle_{\mathrm{QSP}}=\frac{\int\Pi_i\mathcal{D}m_i\cdots\exp(-S_{\mathrm{QSP}})}{\int\Pi_i\mathcal{D}m_i\exp(-S_{\mathrm{QSP}})}. \tag{13}$$

In the spherical model, spin-glass ordering is associated with macroscopic condensation into the eigen state of the exchange matrix **J** with the largest eigenvalue. Then the Lagrange multiplier z ''sticks'' at that eigenvalue and stays constant within SG phase.

Further progress in solving of the model requires diagonalization of the random matrix J_{ij} along with the imposition of the self-consistency constraint (12). The first step is to introduce new variables $m_\lambda(\tau)$ via the relation $m_i(\tau)=\Sigma_\lambda m_\lambda(\tau)\boldsymbol{\psi}_i^\lambda$ using an orthogonal transformation that diagonalizes **J**

$$\sum_i J_{ij}\boldsymbol{\psi}_i^\lambda=\mathcal{J}_\lambda\boldsymbol{\psi}_j^\lambda, \tag{14}$$

where $\lambda=1,\ldots,N$ and $\mathcal{J}_\lambda$ is the λth eigenvalue. The eigenvectors (that are statistical variables) are orthogonal and we can choose them to be normalized,

$$\sum_{i=1}^N \boldsymbol{\psi}_i^\lambda\boldsymbol{\psi}_i^{\lambda'}=0, \quad \text{for } \lambda\neq\lambda', \tag{15}$$

$$\sum_{i=1}^N (\boldsymbol{\psi}_i^\lambda)^2=1. \tag{16}$$

In terms of new variables after transforming to the frequency space Eq. (10) becomes

$$S_{\mathrm{QSP}}[m,z_0]=\frac{1}{2\beta}\sum_{\omega_\ell}\sum_\lambda\left[\mathcal{J}_\lambda-2z_0+\frac{1}{K_{02}(\omega_\ell)}\right]\times m_\lambda(\omega_\ell)m_\lambda(-\omega_\ell)+Nz_0, \tag{17}$$

where $K_{02}(\omega_\ell)=4\Delta\tanh(\beta\Delta)/(4\Delta^2+\omega_\ell^2)$ and $\omega_\ell=2\pi\ell T$, $\ell=0,\pm1,\pm2,\ldots,$ being the Bose Matsubara frequencies. Accordingly, the self-consistency condition (12) reads

$$1=\frac{1}{\beta}\sum_{\omega_\ell}\int dE\frac{\rho(E)}{E-2z_0+1/K_{02}(\omega_\ell)}, \tag{18}$$

where we have used $(1/N)\Sigma_\lambda\to\int dE\rho(E)$ in the limit $N\to\infty$. Here,

$$\rho(E)=\frac{1}{N}\sum_\lambda\overline{\delta(E-\mathcal{J}_\lambda)}=\frac{1}{2\pi J^2}\sqrt{4J^2-E^2}\,\Theta(2J-|E|) \tag{19}$$

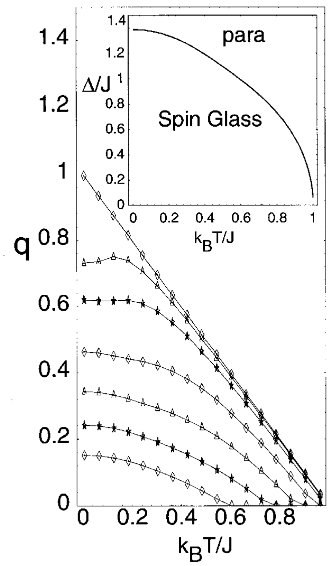

FIG. 1. The spin-glass order parameter q as a function of the temperature for several values of the fixed transverse field $\Delta/J=0$, 0.1, 0.2, 0.4, 0.6, 0.8, and 1 (from the top to the bottom). The inset shows the critical phase boundary $T_{\mathrm{crit}}(\Delta)$ between disordered and spin glass phases for the spherical approximation of the infinite-range interaction quantum Ising spin-glass model in the transverse field.

is the averaged density of states corresponding to the random semicircle law.[16] Finally, summing over Matsubara frequencies the self-consistency Eq. (18) for the Lagrange multiplier z_0 becomes

$$1=\sqrt{\frac{8\Delta\tanh(\beta\Delta)}{J}}\int_{-1}^{1}\frac{dx}{\pi}\sqrt{\frac{1-x^2}{(z_0/J)-x}}\times\left[\frac{1}{2}+f_B\left(J\sqrt{\frac{8\Delta\tanh(\beta\Delta)}{J}}\sqrt{\frac{z_0}{J}-x}\right)\right], \tag{20}$$

where $f_B(y)=1/(e^{\beta y}-1)$ is the Bose distribution function. For $T<T_{\mathrm{crit}}(\Delta)$, where $T_{\mathrm{crit}}(\Delta)$ marks the onset of the SG the saddle point value z_0 is fixed at $z_0=J$ being the branch point of the integrand of Eq. (18). To study the SG order parameter and response functions we introduce into Eq. (10) a source term $-\Sigma_i\int_0^\beta d\tau h_i(\tau)m_i(\tau)$, where $h_i(\tau)$ is the fluctuating field at site i that couples to the ''spin variable'' $m_i(\tau)$. Introducing the SG order parameter

$$q=\frac{1}{N}\sum_\lambda\overline{\langle m_\lambda(\tau)m_\lambda(\tau+0)\rangle}_{\mathrm{QSP}} \tag{21}$$

we obtain the equation of state for the quantum spherical Ising spin glass in a form

$$q=1-\frac{4}{3\pi}\sqrt{\frac{4\Delta\tanh(\beta\Delta)}{J}}\left[1+6\int_0^1 dx\,x\sqrt{1-x^2}f_B\times\left(2Jx\sqrt{\frac{4\Delta\tanh(\beta\Delta)}{J}}\right)\right]. \tag{22}$$

The critical line $T_{\mathrm{crit}}(\Delta)$ results immediately from the substitution $q=0$ in Eq. (22) and is presented [together with

$q(T,\Delta)$ dependence] in Fig. 1. For vanishing of the transverse field the order parameter reads simply $q=1-k_BT/J$ —in agreement with the result of Thouless and Jones for the classical spherical Ising spin glass (see, Refs. 12). We can examine the accuracy of the quantum spherical approximation by referring our results to the previous studies on the quantum infinite-range Ising spin glass in a transverse field (see Refs. 11 and 17 for quantitative comparison of various methods). The agreement with the best numerical calculations is fairly good. For example, the corresponding quantum-critical point in the present approach reads $\Delta_{\rm crit}(T=0)/J=9\pi^2/64\approx 1.3879$ and is very close to the value obtained by extensive numerical Trotter-Suzuki computations (≈ 1.5) and much better than the static approximation [$\Delta_{\rm crit}(T=0)/J=2$]. This justifies the usefulness of the presented ''sphericalization'' technique for quantum disordered systems.

Finally, some comments on the nature of the SG phase in the present model are in order. It is well known that the solution for the classical spherical model shows absence of any instability in the low temperature phase, i.e., in the language of the replica theory the model preserves the replica symmetry.[18] On the other hand the need to break replica symmetry appears already in the classical Ising case[19] below a certain temperature. In the present quantum Ising SG model the replica symmetry breaking solution should occur since the model maps onto the classical Ising system for $\Delta=0$. Although in the related quantized spherical version of the model the replica method was not explicitly used one can easily prove that the solution (22) is replica symmetric and marginally stable. However, this solution might persist only until higher order terms then quadratic in m have been included in the action (17). These terms being a perturbation around spherical model presumably spoil the replica symmetric solution of the quantized spherical model as it happens in its classical counterpart.[20] We are then forced to look for the SG order parameter in a general form of the Parisi replica symmetry breaking scheme. Exploring this possibility remains the subject for further study.

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