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The tricritical point in the quantum Ising $S = 1$ spin glass with biaxial crystal-field effects

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Abstract. We study a quantum generalization of the infinite-range Sherrington–Kirkpatrick spin-glass model with biaxial crystal-field effects described by two uniaxial anisotropy parameters D_x and D_y. For spin dimensionality $S = 1$ we report an analytical and numerical analysis in the (T, D_x, D_y) parameter space (with T being the temperature). For $D \equiv D_x = D_y$ the model effectively becomes classical and identical with the crystal-field-split spin-glass Ising model (introduced by Ghatak and Sherrington) showing a discontinuous phase transition to the spin-glass phase on a portion of the T–D line.

1. Introduction

Various types of anisotropy have a profound influence on the spin-glass (SG) phase of solids. Examples are anisotropies due to the crystal field of the host and non-magnetic impurities which affect the spin interaction symmetries. For example, strong uniaxial anisotropy of the magnetic susceptibility was found experimentally in a number of hexagonal metallic spin-glass systems [1–3] (such as dilute **Zn**Mn, **Cd**Mn and **Mg**Mn) and this has stimulated theoretical research.

From a theoretical point of view, anisotropy gives rise to several new features which have been investigated for classical spin models both with and without a magnetic field, and a multiplicity of phases have been found [4, 5]. The corresponding quantum spin problem can yield results which are qualitatively different from their classical counterparts [6, 7]. For example, when the negative uniaxial anisotropy is large for integer spins at low temperatures, one obtains in the quantum case condensation into a state resulting in a non-magnetic spin phase accompanied by the destruction of the spin-glass character [6], whereas in the classical case the spin-glass phase exists for arbitrary negative value of D [4]. Similarly, for large cubic anisotropy (the sign of which depends on the spin) and for integer spin, the ground state is non-magnetic and the spin-glass order is absent [8]. Recently, anisotropic *biaxial* quantum spin systems have emerged as good candidates for displaying first- or second-order phase transitions around the crossover temperature between the thermal and quantum regimes for the escape rate (depending on the anisotropy constant and the external magnetic field; see references [9]).

In the present paper we consider the properties of a quantum Ising-like model with *biaxial* crystal-field effects. In physical terms, an Ising SG with a biaxial crystal field is described by a

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model in which single-ion uniaxial energies along two axes are added to the random isotropic Ising exchange interaction. As we shall see, the model can exhibit a continuous paramagnet-to-spin-glass transition within the range of crystal-field parameters corresponding to a doublet ground state for an isolated spin, but both continuous and discontinuous transitions for the case of an isolated spin singlet, ground states with a tricritical point separating these transitions.

The Hamiltonian of the model is given by

$$H = -\frac{1}{2}\sum_{i,j=1}^{N} J_{ij} S_i^z S_j^z - \sum_{i=1}^{N}\left[D_x (S_i^x)^2 + D_y (S_i^y)^2\right] \tag{1}$$

where $\boldsymbol{S} = (S_x, S_y, S_z)$ is the quantum spin operator associated with the local moment S at site $i = 1, \ldots, N$. The J_{ij} $(i \neq j)$ are quenched, random exchange interactions governed by independent Gaussian distributions with mean zero and variance $J/\sqrt{N}$. The second term in equation (1) gives rise to uniaxial energy splitting (along the z-direction) for $D_x = D_y$, whereas for $D_x \neq D_y$ there is biaxial anisotropy in the xy-plane. Using $S_x^2 + S_y^2 + S_z^2 = S(S+1)$ we can write the second, single-body term in the Hamiltonian (1) as

$$\begin{aligned} H_0 &= -(D_x S_x^2 + D_y S_y^2) = -D(S_x^2 + S_y^2) - \Delta(S_x^2 - S_y^2) \\ &= DS_z^2 - \Delta(S_x^2 - S_y^2) + DS(S+1) \end{aligned} \tag{2}$$

where

$$D = \frac{1}{2}(D_x + D_y) \qquad \Delta = \frac{1}{2}|D_x - D_y|.$$

In particular, for $\Delta = 0$ the quantum Hamiltonian (1) reduces to the purely classical model

$$H = -\frac{1}{2}\sum_{i,j=1}^{N} J_{ij} S_i^z S_j^z + D\sum_{i=1}^{N}(S_i^z)^2 \tag{3}$$

previously studied by Ghatak and Sherrington [10]. They showed that the model possesses unusual features, manifesting both continuous and first-order phase transitions. Lage and de Almeida [11] and also other groups [12] investigated the stability of the Ghatak–Sherrington solution and have demonstrated a number of subtleties of this model. In the present paper the quantum generalization (1) enables us in particular to recover the Ghatak–Sherrington solution from the extended parameter space $(k_B T, D_x, D_y)$. As in the paper of Ghatak and Sherrington we restrict ourselves to a case corresponding to the lowest non-trivial spin value $S = 1$.

2. Formalism

Determination of the properties of quantum spin glasses is a non-trivial problem due to the non-commutativity of the operators in the Hamiltonian. The addition of quantum fluctuations generally precludes an exact solution—even for the paramagnetic phase—commonly used in the spin-glass theory mean-field limit. A number of studies of various models have shown that the intrinsic difficulty originates from the presence of a dynamical self-interaction induced by averaging over the randomness. This self-interaction plays the role of an order parameter and has to be determined self-consistently—in contrast to the case for classical spin glasses—even in the paramagnetic phase. However, in most cases an attempt to solve this dynamic problem leads even in the simplest approximations to integral equations involving the dynamic self-interaction [13]. As an alternative approach, the Trotter–Suzuki formula [14] may be used, recasting the problem into a classical $d + 1$ equivalent, with long-range interactions. This classical model may then be studied numerically using exact spin summations or Monte Carlo techniques [15]. Unfortunately, this approximation is not able to penetrate the temperature

region close to $T = 0$ and suffers from numerical difficulties with direct spin summations or the so-called negative-sign problem in Monte Carlo calculations for non-Ising models [16]. An approximate analytically tractable solution to the problem can be obtained by replacing the dynamic self-interaction by an appropriate time average. Then, the resulting equations are readily solved and the phase diagrams can be computed. In the context of the Matsubara imaginary-time and replica approach this method is referred to as *the static approximation* [17], while for the real-time thermo-field description we are dealing with the *instantaneous approximation* [18]. While conceptually simple, these approximations offer a first step towards the description of quantum phase transitions in disordered systems, and for many systems with complicated interactions and/or higher dimensions of spin variables they seem to be the only tractable approaches [19]. In this paper we employ the thermo-field dynamics (TFD) method [20]. It is based on a real-time, finite-temperature, quantum field theory, and it is a quantum analogue of the dynamical Martin–Rose–Siggia approach [21] used to deal with classical spin glasses [22]. A detailed procedure for applying the TFD method to spin-glass models has been described in reference [23]. Here we sketch this approach, giving only those points necessary for implementing the method for the case under consideration.

We start from the disorder-averaged generating functional for the real-time finite-temperature causal Green's functions in the form

$$\langle Z[\eta, \{J_{ij}\}]\rangle_J = \int \prod_{ab} \mathrm{D}Q^{ab} \ \exp(-NL[\boldsymbol{Q}] + \Omega[\eta]) \tag{4}$$

where $Z[\eta, \{J_{ij}\}]$ is the unaveraged generating functional for a fixed realization of random bonds and $\Omega[\eta] = \mathrm{Tr}(\boldsymbol{Q}\eta)/J^2$ represents the source term. The effective Lagrangian is

$$L[\boldsymbol{Q}] = \mathrm{Tr}\,\boldsymbol{Q}^2 - \ln \Phi[\boldsymbol{Q}] \tag{5}$$

where

$$\mathrm{Tr}\,\boldsymbol{Q}^2 = \int_{-\infty}^{+\infty} \mathrm{d}t \ \int_{-\infty}^{+\infty} \mathrm{d}t' \sum_{ab} Q^{ab}(t,t')Q^{ba}(t',t)$$

$$\Phi[\boldsymbol{Q}] = \langle O, \beta | T_t U\, Q_0(-\infty;+\infty) | O, \beta\rangle$$

$$U_{Q_0}(-\infty;+\infty) = \exp\left(-\mathrm{i}\int_{-\infty}^{+\infty} \mathrm{d}t \ \int_{-\infty}^{+\infty} \mathrm{d}t' \hat{H}_Q(t,t')\right).$$

Here, the time-ordered exponential results from the interaction picture, and $Q^{ab}(t,t') = Q^{ba}(t',t)$ represents a symmetric time-dependent tensor field. The effective time-dependent single-site thermal Hamiltonian is given by

$$\hat{H}_Q(t,t') = -\sum_{ab} (\epsilon_a \epsilon_b)^{1/2} J\, Q^{ab}(t,t') S_z^a(t) S_z^b(t') \tag{6}$$

where $a, b = 1, 2$ are the TFD 'dynamic replicas' ($\epsilon_1 = 1, \epsilon_2 = -1$) labelling the collective fields $J\,Q^{ab}$ which act as dynamic self-interactions between time-dependent spin operators

$$S_z^a(t) = \exp(-\mathrm{i}H_0 t) S_z^a \exp(\mathrm{i}H_0 t).$$

Finally

$$\langle O, \beta | \cdots | O, \beta\rangle = \mathrm{Tr}\,\mathrm{e}^{-\beta H_0} \cdots / \mathrm{Tr}\,\mathrm{e}^{-\beta H_0}. \tag{7}$$

From equation (6) it can be seen that the quantum generalization of the problem results in a time-dependent self-interaction $J\,Q^{ab}(t,t')$ between spin operators at the same site, which must be

determined self-consistently. In the limit $N \to \infty$, the steepest-descent method can be used, giving the following equation for the stationary-point value of the dynamic self-interaction:

$$Q_0^{ab}(t,t') = \frac{1}{2}(\epsilon_a \epsilon_b)^{1/2} J G^{ab}(t,t') \tag{8}$$

where the causal Green's function is defined as

$$G^{ab}(t,t') = -\mathrm{i}\frac{\langle O,\beta|T_t S_z^a(t) S_z^b(t') U_{Q_0}(-\infty;+\infty)|O,\beta\rangle}{\langle O,\beta|T_t U\, Q_0(-\infty;+\infty)|O,\beta\rangle}. \tag{9}$$

The correspondence with measurable quantities is achieved by decomposing the Fourier transform of $G^{ab}(\omega)$:

$$\begin{aligned} G^{ab}(\omega) &= [\boldsymbol{U}_B(\omega)\hat{\tau}\overline{G}(\omega)\boldsymbol{U}_B(\omega)]^{ab} \\ &= \left[\hat{\tau}\overline{G}(\omega)\right]^{ab} - 2\mathrm{i}\frac{\boldsymbol{C}_{\mathrm{reg}}(\omega)}{\mathrm{e}^{\beta\omega}+1}\begin{bmatrix} 1 & \mathrm{e}^{\beta\omega/2} \\ \mathrm{e}^{\beta\omega/2} & 1 \end{bmatrix} + G^{ab}_{\mathrm{sing}}(\omega). \end{aligned} \tag{10}$$

Here $\boldsymbol{U}_B(\omega)$ is the thermal transformation matrix [24], while $\overline{G}^{ab}(\omega)$ is the matrix of retarded (advanced) $G_{R\,(A)}(\omega)$ Green's functions:

$$\overline{G}^{ab}(\omega) = \begin{bmatrix} G_R(\omega) & 0 \\ 0 & G_A(\omega) \end{bmatrix} \tag{11}$$

and

$$\hat{\tau} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{12}$$

The quantity $\boldsymbol{C}_{\mathrm{reg}}(\omega)$ in equation (10) refers to the matrix of the thermodynamic correlation functions in the spin-component space which is related to $G^R(\omega)$ by means of the fluctuation-dissipation theorem. Furthermore, it turns out that the time-persistent part $G^R_{\mathrm{sing}}(\omega)$ has the form

$$G^{ab}_{\mathrm{sing}}(\omega) = -2\pi\mathrm{i}q\delta(\omega)\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}^{ab} \tag{13}$$

where q is the Edwards–Anderson [25] spin-glass order parameter which is non-zero in the spin-glass phase.

3. Determination of critical lines

The location of the spin-glass transition can be described by the condition $q = 0$ or, equivalently, by the divergence of the inverse relaxation rate [22] characterized by a generalized damping function $\gamma(\omega)$, defined as

$$\gamma^{-1}(\omega) = \mathrm{i}\frac{\partial G_R^{-1}(\omega)}{\partial\omega} \tag{14}$$

which diverges in the static limit ($\omega \to 0$) along the critical line. The condition for divergence of the damping function γ^{-1} is

$$1 = J\chi \tag{15}$$

where

$$\chi = \lim_{\omega\to 0} G_R(\omega) = \lim_{\omega\to 0} G_A(\omega). \tag{16}$$

Because of the appearance of the dynamic self-interaction $J\,Q^{ab}(\omega)$ in the effective thermal Hamiltonian (6), the evaluation of equation (9) is difficult. For the quantum spin-glass problem

an exact calculation of the transition lines requires precise knowledge of the time dependence of the dynamic spin self-interaction involved. This means that the calculation of the exact phase boundary will depend on the detailed time dependence of $Q^{ab}(t)$ (and, correspondingly, the analogous quantity in the 'imaginary-time' Matsubara approach with the replica method). For this reason we focus on the effects of quantum fluctuations on a timescale such that the finite-time part of the dynamic self-interaction can be represented by an instantaneous term† which simplifies the time dependence of $Q^{ab}(t)$:

$$Q^{ab}(t-t') = \frac{1}{2}(\epsilon_a\epsilon_b)^{1/2} J\chi\delta(t-t')\delta_{ab}. \tag{17}$$

It seems that the complexity of the problem (in particular the spin value greater than $S = 1/2$) prevents an analytically tractable approach which goes beyond the *ansatz* (17). In the above-mentioned Matsubara method, usually one resorts to similar simplifications—for example, discarding the 'imaginary-time' dependence of the dynamic self-interaction (the so-called static approximation). As was pointed out elsewhere [28], the static and instantaneous approximations will give rough upper and lower bounds, respectively, for the critical line. Therefore, the exact phase boundary should be located in the region between two curves corresponding to the above-mentioned approximations. It is also interesting to note that the phase boundaries determined by the two methods become closer together as the spin value S increases [8]. (For a detailed comparison and discussion of both Matsubara and TFD approaches as well as other methods in the context of quantum spin-glass models, we refer the interested reader to references [28, 29].)

Within the approximation given by equation (17), the effective single-site quantum spin Hamiltonian becomes

$$H_{\text{eff}}(\xi) = -\frac{1}{2}J^2\chi S_z^2 - (D_x S_x^2 + D_y S_y^2) - J\xi\sqrt{q}S_z \tag{18}$$

and contains the order parameter q and the susceptibility χ which, in turn, are the solutions of the system of equations

$$q = q\mathrm{e}^{J^2\beta\chi}\int_{-\infty}^{+\infty}\frac{\mathrm{d}\xi}{\sqrt{2\pi}}\,\mathrm{e}^{-\xi^2/2}\frac{(2J\xi)^2}{\Delta^2+J^2q\xi^2}\left[\frac{\sinh(\beta\sqrt{\Delta^2+J^2q\xi^2})}{\mathrm{e}^{\beta D}+2\mathrm{e}^{(1/2)J^2\beta\chi}\cosh(\beta\sqrt{\Delta^2+J^2q\xi^2})}\right]^2 \tag{19}$$

$$\chi = 2\mathrm{e}^{J^2\beta\chi}\int_{-\infty}^{+\infty}\frac{\mathrm{d}\xi}{\sqrt{2\pi}}\,\mathrm{e}^{-\xi^2/2}\left\{\frac{\Delta^2\sinh(\beta\sqrt{\Delta^2+J^2q\xi^2})}{(\Delta^2+J^2q\xi^2)^{3/2}[\mathrm{e}^{\beta D}+2\mathrm{e}^{(1/2)J^2\beta\chi}\cosh(\beta\sqrt{\Delta^2+J^2q\xi^2})]}\right.$$
$$\left.+\frac{q\beta J^2[2\mathrm{e}^{(1/2)J^2\beta\chi}+\mathrm{e}^{\beta D}\cosh(\beta\sqrt{\Delta^2+J^2q\xi^2})]}{(\Delta^2+J^2q\xi^2)[\mathrm{e}^{\beta D}+2\mathrm{e}^{(1/2)J^2\beta\chi}\cosh(\beta\sqrt{\Delta^2+J^2q\xi^2})]^2}\right\}. \tag{20}$$

The critical line is given by the equation $1 = J\chi$ (equation (15)) with $q = 0$, and from equation (20) we obtain

$$2\beta D = \ln\left\{2\left[\beta J\frac{\sinh(\beta\Delta)}{(\beta\Delta)} - \cosh(\beta\Delta)\right]\right\}. \tag{21}$$

The corresponding phase diagram in the parameter space is presented in figure 1 (k_BT, D_x, D_y) and the anisotropy–temperature dependences of the related quantities, namely χ and q, are given for $D_x = D_y$ in figure 2 and for $D_x \neq D_y$ in figure 3. The k_BT–D_x–D_y surface in

† Here, the finite-time term $Q^{ab}(t-t')$ in the instantaneous approximation corresponds to the replica-diagonal order parameter p in the formulation of Ghatak and Sherrington (which gives a non-trivial quadrupolar contribution), in contrast to q which is given by the static time-independent quantity in the dynamic approach (and corresponds to the replica-off-diagonal contribution in the replica formalism).

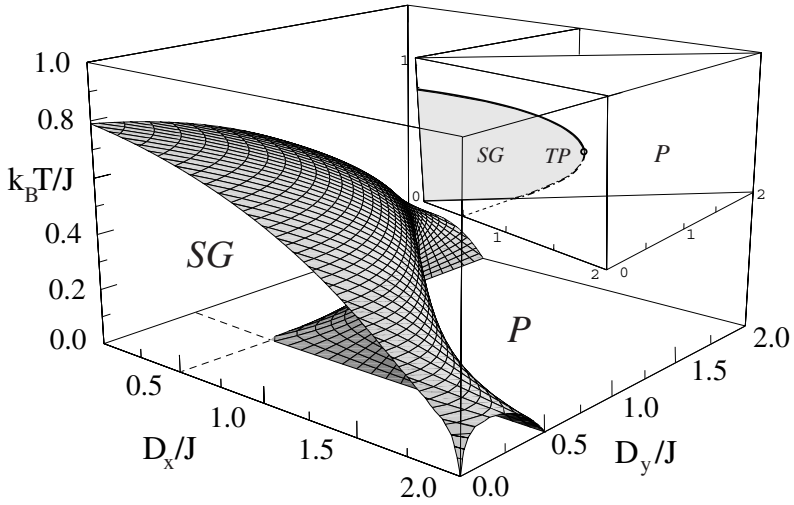

Figure 1. The phase diagram with $S = 1$ for the biaxial anisotropy and temperature (D_x, D_y, T). The surface separates the spin-glass (SG) phase from the paramagnetic region (P). The inset shows the critical line for $D_x = D_y$ when the quantum model reduces to the classical one with uniaxial anisotropy. The tricritical point (TP) separates continuous and discontinuous (broken line) transitions between SG and P phases.

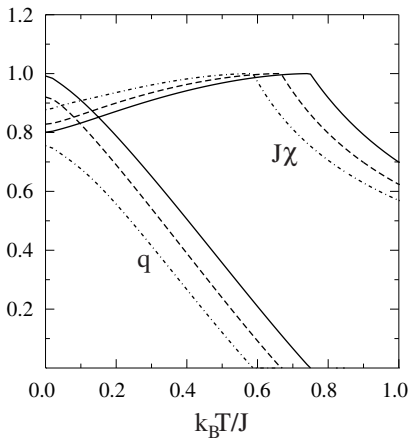

Figure 2. The susceptibility (χ) and the order parameter (q) as functions of the temperature (T) for various uniaxial anisotropies $D_x = D_y = D$: $D = 0.2$ (solid line), $D = 0.5$ (dashed line) and $D = 0.7$ (dashed–dotted line).

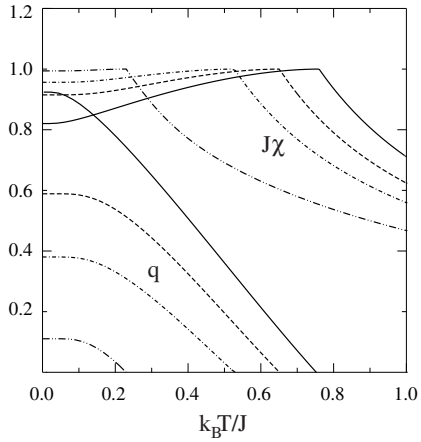

Figure 3. The susceptibility (χ) and the order parameter (q) as functions of the temperature (T) for various biaxial anisotropies $D_x \neq D_y = 0.1$: $D_x = 0.2$ (solid line), $D_x = 0.8$ (dashed line), $D = 1.2$ (dashed–dotted line) and $D_x = 1.8$ (dashed–double-dotted line).

figure 1 represents the locus of the continuous phase transition except for that portion of the line (resulting from the cut of the surface by the plane $D_x - D_y = 0$ where the phase transition occurs with a discontinuous change of χ and q) which ends with the tricritical point—this is precisely the line found by Ghatak and Sherrington† for the model (3).

† The self-consistent equations (19) and (20) for q and χ reduce in the limit $D_x \to D_y \equiv D$ (classical case) exactly to those found by Ghatak and Sherrington using the replica method on observing that $\chi = \beta(p - q)$, where p is the replica-diagonal order (quadrupolar) parameter introduced by Ghatak and Sherrington.

4. Summary and final remarks

We have studied the case of a quantum Ising spin glass with $S = 1$ (representative of the integer-valued spin models) with biaxial crystal-field effects. We determined the critical surface in the three-dimensional parameter space (J, D_x, D_y) (see (1)) and discussed the relationship of the quantum model to the related classical system (for a particular choice of the biaxial anisotropy parameters) studied by Ghatak and Sherrington. It should be pointed out that the solutions for the order parameter and susceptibility *within* the spin-glass phase are only approximate, as replica-symmetry-equivalent solutions are always unstable and unsatisfactory.

The unresolved issue in this work is the construction of the replica-symmetry-breaking (RSB) solution for a quantum SG model studied here. Generally, it is accepted that RSB can be interpreted as a factorization of the phase space into an (ultrametric) hierarchy of 'valleys' or pure states separated by macroscopic barriers. For systems with discontinuous SG transitions, an effective factorization of the phase space into a finite number of pure states is expected, making the strong non-ergodic continuous RSB less probable as compared to the single-step RSB which might survive. It would also be interesting to see whether the full Parisi treatment will alter the location of the first-order transition line. We hope to address the stability problem in a future paper. Finally, it is evident that the model studied here is not yet sufficiently close to real spin-glass systems. The effects of random anisotropy, net ferromagnetic interaction and finite-dimensionality effects require further study.

Acknowledgment

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Here different approximations (including TFD and the Matsubara method) are compared with more rigorous treatment of the dynamic self-interaction based on the Green's function and the Trotter–Suzuki method.