Effects of anisotropy on a quantum Heisenberg spin glass on a three-dimensional hierarchical lattice

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We study the anisotropic Heisenberg spin-glass model on a three-dimensional hierarchical lattice (designed to approximate the cubic lattice), within a real-space renormalization-group approach. Two different initial probability distributions for the exchange interaction (J_{ij}), Gaussian and uniform, are used, with zero mean and width $\overline{J}$. The $(kT/\overline{J})\times\Delta_0$ phase diagram is obtained, where T is the temperature, Δ_0 is the first moment of the probability distribution for the uniaxial anisotropy, and k is the Boltzmann constant. For the Ising model ($\Delta_0=1$), there is a spin-glass phase at low temperatures (high $\overline{J}$) and a paramagnetic phase at high temperatures (low $\overline{J}$). For the isotropic Heisenberg model ($\Delta_0=0$), our results indicate no spin-glass phase at finite temperatures. The transition temperature between the spin-glass and paramagnetic phase decreases with Δ_0, as expected, but goes to zero at a finite value of the anisotropy parameter, namely $\Delta_0=\Delta_c\sim 0.59$. Our results indicate that the whole transition line, between the paramagnetic and the spin-glass phases, for $\Delta_c<\Delta_0<1$, belongs to the same universality class as the transition for the Ising spin glass.

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I. INTRODUCTION

Considerable attention during the past decade has been devoted to the investigation of systems displaying spin-glass (SG) order. Numerical studies [1] have revealed that the SG phase transition occurs in the three-dimensional Ising model (strongly anisotropic system), indicating that the lower critical dimension for the Ising SG would be $d_l=2$. On the other hand, many real materials that show SG order are Heisenberg-like rather than Ising-like, in the sense that the magnetic anisotropy is considerably weaker than the isotropic exchange interaction. Some Monte Carlo simulations [2,3] have indicated that the isotropic three-dimensional classical Heisenberg SG with finite-range interaction does not exhibit the conventional SG order at finite temperatures in zero field, while Lee and Young [4] found such an ordered phase at finite temperatures for this model.

Experiments clearly demonstrate the existence of order at finite temperatures in Heisenberg-like SG systems [5], where the chirality-driven mechanism proposed by Kawamura [3,6] can be interpreted consistently to explain some of the puzzles concerning the experimentally observed SG transition in zero field [5]. Note that the numerical observation of a finite-temperature chiral-glass (CG) transition ($T_{CG}>0$) in the three-dimensional classical Heisenberg SG is not inconsistent with the earlier observation of the absence of the conventional SG order at finite temperatures ($T_c=0$). In Refs. [3,6] it is suggested that the SG-paramagnetic critical temperature obeys $T_c<T_{CG}$, and quite possibly $T_c=0$ in three dimensions. In the presence of a small random magnetic anisotropy, which always exists in real experimental situations, an SG phase is expected to emerge as a result of the fact that the anisotropy mixes the two degrees of freedom, spin and chirality. Therefore, in the chirality-driven mechanism the SG phase transition experimentally observed in a class of compounds such as CuMn is essentially governed by the CG fixed point.

Note, however, that some numerical results support that the SG transition temperature might coincide with the CG transition temperature, i.e., $T_c=T_{CG}>0$ [4,7], in contrast with the results of Refs. [3,6] (which show that in three dimensions the spin and the chirality are decoupled on sufficiently long length scales, with $T_c<T_{CG}$). Therefore, the presence of SG order in the three-dimensional short-range Heisenberg SG is still an open question. In four or more dimensions, there is numerical evidence of a phase transition [8], and so the lower critical dimension d_l for the short-range Heisenberg spin glass should satisfy $3\leqslant d_l<4$.

On the other hand, various types of anisotropies have a profound influence on the SG phase such as Dzyaloshinski-Moriya (DM), dipolar coupling, and uniaxial. A weak anisotropy is crucially important in realizing a finite-temperature SG transition, which causes a crossover from the isotropic Heisenberg behavior to the anisotropic Ising behavior. The expected Heisenberg-to-Ising crossover, however, has not been observed experimentally, and this puzzle has remained unexplained. Using a hybrid Monte Carlo method in the short-range $\pm J$ Heisenberg spin glass with random anisotropy of a DM type (D) on a simple cubic lattice [9], it has been shown that for small values of D, the transition temperature vanishes as $T_c/J\simeq 0.53(D/J)^{1/4}$. This result is consistent with those found by Morris *et al.* [10] based on a

scaling argument. When the spin interactions are of long-range Ruderman-Kittel-Kasuya-Yoshida (RKKY) type, the critical temperature has a much weaker dependence on the anisotropy, namely $T_c/J \simeq [\ln(J/D)]^{-1/2}$ $(D \ll < J)$ [11]. These two studies indicate that in the isotropic limit $(D=0)$ there is no SG order at finite temperatures, i.e., $T_c=0$. However, this result has recently been challenged [4]. To the best of our knowledge, the only previous work on a spin-glass model with uniaxial anisotropy is the one by Matsubara *et al.* [12], where it is speculated that this anisotropy does not lead to an SG phase at finite temperatures.

Another question, which is particularly significant, is the study of quantum effects in the theory of spin glasses [13]. From the theoretical point of view, it is well known that quantum spin glasses, in comparison with their classical counterparts, are far from being trivial, due to the noncommutativity of the spin operators involved (see, for example, the discussion for the quantum transverse Ising SG model with short- and long-range interactions, in Refs. [14,15], respectively). In the limit of very low temperatures the role of quantum fluctuations in pure or disordered systems becomes more and more important. At the critical point itself, fluctuations exist over all scales. At moderate temperatures, quantum fluctuations are usually suppressed in comparison with thermal ones. At low temperatures, however, quantum fluctuations, especially in low-lying states, may dominate and strongly influence the critical behavior of the system. There are a few works on quantum Heisenberg SG, but only infinite-range-interaction models have been treated [16].

Our motivation for this work is the well known fact that the anisotropy may change the nature of phase transitions in a fundamental way, and may induce the appearance of an SG phase in the three-dimensional short-range Heisenberg model. Also, the quantum influence in the phase diagram is a matter of intrinsic interest, particularly from the experimental point of view, with relation to high-temperature superconductor materials [17]. Aharony *et al.* [18] suggested a mechanism in which doping by holes introduces ferromagnetic bonds into an otherwise antiferromagnetic quantum spin-$1/2$ Heisenberg model. These holes are localized in the insulating antiferromagnetic phase and their effect can be well approximated by a quenched random distribution of ferromagnetic bonds which display an SG phase at low temperatures, as a window between the insulating antiferromagnetic phase and the superconducting phase. Physically, the SG phase in this new superconductor compound is attributed to the presence of the random Dzyaloshinski-Moriya interaction [18]. We will show in this work that the presence of uniaxial anisotropy induces an SG phase at low temperatures only for a finite value of the anisotropy; for small enough values of the anisotropy, no long-range SG order is observed, which confirm the results of Mastubara *et al.* [12].

II. METHOD

The main issue we want to address is the influence of a uniaxial anisotropy on the phase diagram of the quantum Heisenberg spin-glass, with Hamiltonian,

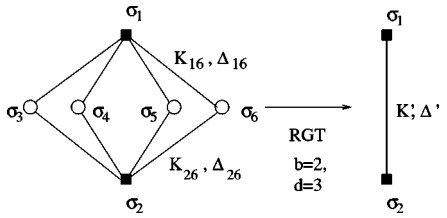

FIG. 1. Hierarchical lattice suitable for calculating the renormalization-group transformations on the simple cubic lattice. The calculation of the renormalized quantities (right-hand side of the figure) is explained in the text.

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij}[(1-\Delta_{ij})(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) + \sigma_i^z \sigma_j^z],$$

where σ_i^α is the component α of a spin-$1/2$ Pauli matrix in site i and the sum is over all first-neighbor bonds on a cubic lattice. In this work, we study two different initial probability distributions for J_{ij}, a Gaussian and a uniform one, respectively,

$$\mathcal{P}(J_{ij}) = \frac{1}{\sqrt{2\pi \overline{J}}} \exp(-J_{ij}^2/2\overline{J^2}),$$

or

$$\mathcal{P}(J_{ij}) = \begin{cases} \dfrac{1}{2\sqrt{3\overline{J}}}, & -\sqrt{3\overline{J}} < J_{ij} < \sqrt{3\overline{J}}, \\ 0, & \text{otherwise}, \end{cases}$$

where $\overline{J}$ is the width of the distributions. On the other hand, the probability distribution for Δ_{ij} is, *initially*, given by

$$\mathcal{P}(\Delta_{ij}) = \delta(\Delta_{ij} - \Delta_0).$$

We use a real-space renormalization-group approach; this method has been successfully applied in the study of both classical and quantum models. The formalism is especially suitable to obtain multidimensional phase diagrams and qualitative results, indicating universality classes and possible crossover phenomena. A great variety of RG methods has been proposed [19,20] over the past years and applied with success in many different quantum systems [21,22]. Recently, an important simplification of the successful method introduced in Ref. [19] has been proposed [23]; we will develop even further this approach in this work.

Within the context of a small-cell approximation, the simple cubic lattice is represented by a hierarchical one [24], depicted in Fig. 1. The use of this particular hierarchical lattice is equivalent to a Migdal-Kadanoff approximation [25]. The original lattice is shown on the left-hand side of Fig. 1, with different interactions $K_{ij} \equiv J_{ij}/k_B T$ and anisotropy parameters Δ_{ij} between first-neighbor spins σ_i and σ_j. Performing a partial trace over spins σ_3, σ_4, σ_5, and σ_6, we obtain a renormalized Hamiltonian, with parameters K'_{ij} and Δ'_{ij} (right-hand side of Fig. 1).

First, we have to calculate the renormalized distributions (forcing back the distributions to their original shapes leads to wrong results [26]). To do so, we choose the eight interaction parameters for the original lattice, K_{ij}, from the original distribution, while all Δ_{ij} are the same, *initially*; then we calculate the renormalized K' and Δ'. This is done a number of times (usually of the order of 1 million), to get new probability distributions for K' and Δ'. The anisotropy parameter, although uniform in the first iteration of the renormalization group, follows a disordered probability distribution, afterwards. Also, the distribution for K' is no longer the same as the initial one. For the second iteration, we choose K'_{ij} and Δ'_{ij} from the renormalized distributions obtained in the first iteration, combine them as in the left-hand side of Fig. 1, and then calculate K'' and Δ'', i.e., the renormalized quantities for the second iteration. This process is repeated until we reach a "fixed-point" distribution. Alternatively, we can choose to follow the distribution functions for K and $K^{xy} \equiv K(1-\Delta)$; we will compare below the results for both procedures.

For each set of K_{ij} and Δ_{ij}, the renormalized quantities are calculated as follows. Given a set of parameters, chosen from a given probability distribution, we impose that

$$\langle m_1 m_2 | \rho' | m_1 m_2 \rangle = \mathrm{Tr}' \langle \{m\} | \rho(\{K, \Delta\}) | \{m\} \rangle,$$

where $|\{m\}\rangle$ stands for $|m_1 m_2 m_3 m_4 m_5 m_6\rangle$ (and in a similar way for the "bra"), $\rho(\rho')$ is the density matrix of the original (renormalized) cell (ρ' is a function of the renormalized parameters K', Δ', and C'), m_i is the eigenvalue of the σ^z operator at site i, Tr' means a partial trace over spins σ_3, σ_4, σ_5, and σ_6, and $\{K, \Delta\}$ stands for all sixteen parameters in the original cell. Only three elements of ρ' are nonzero, and this is the number of renormalized quantities: K'_{ij}, Δ'_{ij}, and C' (C' is a constant generated by the renormalization procedure which is not relevant for obtaining the phase diagram). So, no extra equation is needed and the procedure is exact at the cluster level. One great advantage of this approach is that no expansion of the Hamiltonian is necessary; this expansion becomes cumbersome if cells with more sites are employed or if models with spin 1 or greater are treated. Moreover, our procedure recovers the same recursion relations as former treatments [19].

III. RESULTS AND DISCUSSION

Our goal is to obtain the $(kT/\overline{J}) \times \Delta_0$ phase diagram. We start from many different points in this diagram and follow the renormalized distributions until a given attractor is reached. In Fig. 2 this phase diagram is depicted: *SG* stands for the spin-glass phase while *P* stands for the paramagnetic one. We expect the spin-glass phase, which is certainly present for the Ising model ($\Delta_0 = 1$) [26], to extend for smaller values of Δ_0. This is the case but notice that the transition line goes to zero at a value of Δ_0 greater than zero. This behavior is analogous to the one for the antiferromagnetic anisotropic Heisenberg model on the square lattice [22], except that in the latter model a reentrant behavior is obtained. The fact that the transition line does not extend to $\Delta_0 = 0$ is usually due to quantum fluctuations which, at low temperatures, are important and, together with thermal fluctuations, tend to drive the system to a disordered phase.

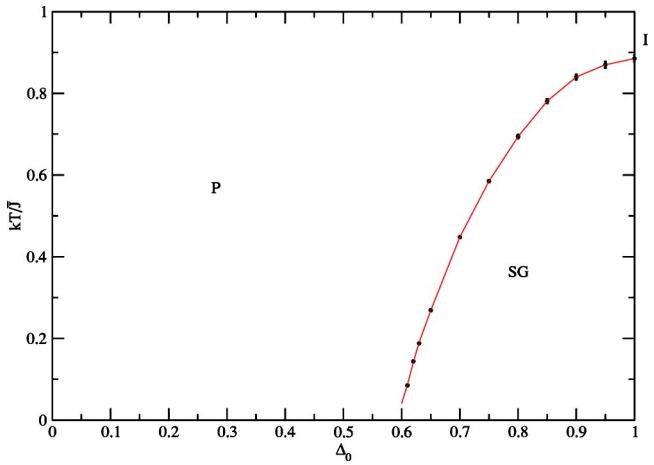

FIG. 2. Approximate phase diagram for the anisotropic Heisenberg spin-glass on the cubic lattice. *SG* stands for the spin-glass phase, *P* stands for the paramagnetic phase, and *I* stands for the Ising transition point. The continuous line is a guide to the eye.

For the Ising subspace ($\Delta_0 = 1$) the fixed-point distribution for the paramagnetic phase attractor is such that $\overline{J}/kT = 0$, while for the SG attractor, $\overline{J}/kT = \infty$. There are still possible fixed points at the line $\Delta_0 = 0$ (isotropic Heisenberg spin glass) but they were not found in this work (see below). For any $\Delta_0 \neq 0$, the attractor is found to be at the line $\Delta_0 = 1$, that is, any initial point with $\Delta_0 \neq 0$ flows, upon application of the renormalization-group procedure, to the $\Delta_0 = 1$ subspace. Exactly at the transition line, the flow is towards the Ising "fixed-point" (point *I* in Fig. 2) and the whole line is attracted to the distribution at that point. Physically, this means that the critical behavior along the line is the same as for the Ising spin glass. Critical exponents for the Ising spin glass are the same as those calculated in Ref. [27]; moreover, the critical probability distribution is the same as in the cited reference, for both Gaussian and uniform probability distributions.

Some points are worth mentioning here. The distributions for K_{ij} and Δ_{ij}, after the first iteration, do not retain its original form. Therefore, a more complete picture of this problem would involve a flux on a space of probability distributions. The phase diagram we chose to represent our results is only a schematic one. On the other hand, if Δ_0 is different from 0 and 1, its distribution after the first iterations is not uniform anymore. It evolves along the renormalization-group procedure and only when the number of iterations increases, the distribution for Δ is again a delta function, $\mathcal{P}(\Delta_{ij}) = \delta(\Delta_{ij} - \Delta_0)$, with $\Delta_0 = 1$ and zero width.

The phase diagram (Fig. 2) shows that there is no spin-glass phase for the isotropic spin-1/2 Heisenberg model in three dimensions. This result confirms those found in earlier works [9,28], indicating that the lower critical dimension for the isotropic spin-1/2 Heisenberg spin glass is greater than three. On the other hand, Lee and Young [4] found a spin-glass phase for the *classical* 3D isotropic Heisenberg model. As the transition takes place at low temperature, it is possible

that quantum fluctuations, present for the spin-1/2 model, are strong enough to eliminate the spin-glass phase. We also find that an infinitesimal uniaxial anisotropy is not able to create an SG phase in a Heisenberg spin-1/2 system, in three dimensions; this is consistent with the findings of Ref. [12].

Our results are qualitatively the same for both Gaussian and uniform distributions. We have also used a correlated distribution for K_{ij} and Δ_{ij} [29] and the results suffer only minor changes, maintaining the overall behavior. In another approach we followed, the probability distributions for the interactions K_{ij} and K_{ij}^{xy} were followed; again, the qualitative behavior is the same as when we follow the distributions for K_{ij} and Δ_{ij}.

Finally, let us mention that, contrary to what happens for systems where only ferromagnetic (or antiferromagnetic) interactions are present [19], there is a strong difference between treating the cell "as a whole" or "by pieces." In the latter, the original cell (see Fig. 1) is seen as a combination in parallel of 4 interactions, each one made of two interactions in series. In this way, the renormalized interaction and anisotropy can be first calculated for each combination in series and then combined in parallel. For systems with no frustration [19], this is shown to introduce an error smaller than 10%, when compared to treating the eight bonds and six spins of the cell "as a whole." This is no longer the case for the model we study here and the errors are much bigger. We believe that, for any system in which frustration is present, the RG procedure has to be done using the whole cell. This is due to the fact that frustration is not taken into account when the cell is renormalized by pieces.

IV. SUMMARY

We applied a quantum renormalization-group procedure to the anisotropic three-dimensional spin-1/2 Heisenberg spin glass. A Migdal-Kadanoff approximation is used and the $(kT/\overline{J})\times\Delta_0$ phase diagram is calculated. The spin-glass phase, present for the Ising model ($\Delta_0=1$), extends to smaller values of the anisotropy parameter. The transition temperature, which separates the ferromagnetic and paramagnetic phases, goes to zero at approximately $\Delta_0=0.59$. According to the approximation we used, the isotropic spin-1/2 quantum Heisenberg spin-glass has no spin glass phase at finite temperature. The whole transition line between the SG phase and the paramagnetic one is found to belong to the same universality class of the three-dimensional Ising spin glass. Our conclusions hold true for Gaussian and uniform distributions, for correlated distributions, and when the probability distributions for (K_{ij},Δ_{ij}) or (K_{ij},K_{ij}^{xy}) are renormalized.

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