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Ground State of the Three-Dimensional Quantum RKKY Spin Glass

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The ground-state properties of the spin-1/2 RKKY Heisenberg spin glass are investigated on the fcc lattice. Numerical diagonalization of finite-size systems and extrapolation to the infinite system suggest either that the correlation function decays in a power law $\langle S_0 \cdot S_r \rangle^2 \sim r^{-1-\eta}$ ($\eta = 0.02 \pm 0.09$) or that there is a small but finite value of the order parameter. From comparison with other theories, we prefer the former possibility of vanishing spin glass ordering.

The three-dimensional Ising spin glass is now believed to have a finite transition temperature.[1~3] In contrast, the random-bond classical Heisenberg model does not undergo a phase transition in three dimensions even if the interaction is of RKKY type.[4,5] The experimental observation of the spin-glass phase[6] is thus explained by a crossover to the Ising universality class by anisotropy.[7] One of the remaining problems is the determination of how quantum effects modify these predictions on classical spin glasses in three dimensions. No reliable information has been obtained on this subject because of a number of difficulties in treating random quantum systems. The present letter represents the first quantitative investigation on the ground-state ordering of RKKY quantum spin systems.

Our model consists of N spin-1/2 Heisenberg spins distributed randomly on the fcc lattice, with the coupling of the RKKY form. The Hamiltonian is given by

$$H = -2 \sum J_{ij} S_i \cdot S_j,$$

where J_{ij} is the RKKY interaction

$$J_{ij} = -J_0 \cos(2k_F r_{ij}) / r_{ij}^3.$$

This Hamiltonian was diagonalized numerically at $T=0$ for finite-size systems up to the number of spins $N=14$. The number of lattice sites for a given N was determined such that the spin concentration of magnetic site is 0.1 atomic%. Fermi wave number k_F of the host metal was chosen as $k_F = 4.91$, which corresponds to half-filling of the conduction band. We calculated the ground-state energy and the order parameter Q defined by

$$Q = 2[\sum \langle S_i \cdot S_j \rangle^2] / N(N-1),$$

where the inner brackets $\langle \ \rangle$ denote the quantum-mechanical average and the outer ones [ ] represent the configurational average with respect to 1000 random selections of magnetic sites. The results are listed in Table I.

Simple extrapolation to the infinite system $N \to \infty$ of the ground-state energy is possible as shown in Fig. 1. The result is

$$E_0 / J_0 N = -0.05 \pm 0.02.$$

The order parameter Q should be extrapolated with sufficient care. If a finite spin-glass ordering exists in the infinite system at $T=0$, Q would approach a finite value as N increases. Then we may fit the data to the functional form

$$Q_1 = a_1 + b_1/N + c_1/N^2.$$

The best fit was found as $a_1 = 0.014 \pm 0.002$,

Table I. The order parameter Q and the ground-state energy E_0/J_0N averaged over 1000 random configurations.

N	Q	E_0/J_0N
6	0.08891 ± 0.00061	-0.0462 ± 0.0035
8	0.06801 ± 0.00036	-0.0507 ± 0.0030
10	0.05519 ± 0.00026	-0.0476 ± 0.0026
12	0.04790 ± 0.00022	-0.0414 ± 0.0022
14	0.04278 ± 0.00021	-0.0418 ± 0.0022

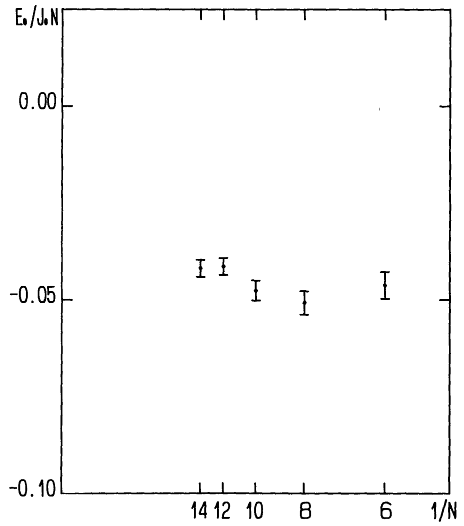

Fig. 1. Ground-state energy versus inverse of the system size. We estimate $E_0/J_0N = -0.05 \pm 0.02$ by simple extrapolation to $N \to \infty$.

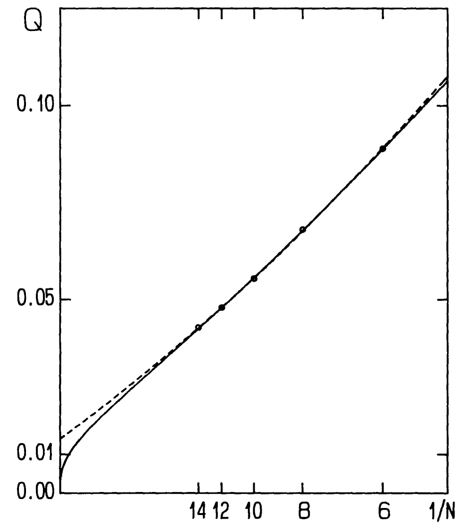

Fig. 2. Order parameter Q as a function of inverse of the system size N. The statistical errors are as small as the dots. The dashed curve shows the fitting function Q_1, and the solid curve is Q_2. There are no distinguishable differences between these two in the range we calculated, $N \leqq 14$.

$b_1 = 0.4 \pm 0.2$, and $c_1 = 0.5 \pm 0.2$. On the other hand, if the correlation function $C_r = [\langle S_0 \cdot S_r \rangle^2]$ decays by a power law $C_r \sim r^{-1-\eta}$, Q is expected to have its N dependence as

$$Q_2 = N^{-a_2}(b_2 + c_2/N).$$

As derived by integrating C_r, a_2 is related to η by $\eta = 3a_2 - 1$. For this case, the finite-size data are best explained by $a_2 = 0.34 \pm 0.03$, $b_2 = 0.060 \pm 0.009$, and $c_2 = 0.62 \pm 0.02$. These two fitting functions, Q_1 and Q_2, are shown in Fig. 2.

The fitting forms Q_1 and Q_2 are of almost the same quality in explaining finite-size data of $N \leqq 14$ (see Fig. 2.) In fact, Fig. 2 shows that the system size (the number of spins N) must be much larger than the present values ($N \leqq 14$) to clearly distinguish Q_1 from Q_2. Thus, it is impossible to determine whether or not a finite spin-glass ordering exists in the ground state as long as one takes into account only the present data. However, the corresponding classical system is likely to have a critical point only at $T = 0$.[4,5,7] More precisely, evidence has been given that the classical RKKY Heisenberg model has the lower critical dimension of three. In this connection, it is useful to remember that a quantum spin system at its lower critical dimension often does not have a finite long-range order at $T = 0$.[8] Therefore, we may conclude that the second possibility, Q_2, is more plausible than Q_1. This readily implies that the correlation exponent η is 0.02 ± 0.09 for this system. Even if a finite long-range order remains, the extrapolated value $a_1 = 0.014 \pm 0.002$ is very small as compared with the value $1/16 = 0.0625$ for full ferromagnetic ordering.

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