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Ground State of Quantum Spin Glass with Infinite Range Interactions

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We have investigated the spin-1/2 random Heisenberg model with infinite range interactions by a numerical method. Extrapolation of finite size ($N \leqq 16$) properties to the infinite system has yielded the following results. The average ground state energy is lower than that of the SK model (Ising spin) by about 25%. In the ground state, a critical point between the spin glass and ferromagnetic (mixed) phases exists just around the critical point ($\tilde{J}_0/\tilde{J}=1$) of the corresponding classical random Heisenberg model. Quantum fluctuations are concluded not to change the ground state properties qualitatively.

§1. Introduction

Magnetic systems with random frozen spins are called spin glasses. Experimental characterization of spin glasses includes[1] a sharp cusp in susceptibility at a certain temperature T_g, hysteresis of magnetization in external fields, and anomalous long relaxation time below T_g. Theoretical efforts to account for these and other experimental observations were initiated by Edwards and Anderson[2] and Sherrington and Kirkpatrick.[3] The Ising model with random infinite range interactions proposed by the latter authors (the SK model) was later solved by Parisi using a replica symmetry breaking scheme.[4] Physical interpretation[5] of his solution revealed a close relationship between the replica symmetry breaking as a mathematical trick to solve the problem and the irreversibility inherent in spin glasses. A solution of the classical Heisenberg spin glass[6] predicted a new phase (the mixed phase) where transverse spin components are randomly frozen while longitudinal components are ferromagnetically ordered. These developments in the mean field theory of classical spin glasses stimulated Bray and Moore[7] to predict a finite transition temperature to a spin glass state in the quantum Heisenberg model with random infinite range interactions. However difficulties in properly treating quantum effects have prevented further progress in the quantum theory of spin glasses.

In these contexts we have investigated the ground state of the quantum Heisenberg spin glass by numerically diagonalizing finite size systems ($N \leqq 16$). All bonds are assumed to be equivalent for the purpose of comparison with mean field predictions on classical systems. Extrapolation of finite size results to the infinite system has yielded the ground state energy and order parameters as functions of the center of distribution $\tilde{J}_0/\tilde{J}$ of exchange interactions. It should be noted that a similar numerical study[8] of the SK model has provided useful information on low temperature properties of the system. Our calculations are limited to the ground state because of insurmountable difficulties in numerically obtaining many eigenvalues and eigenstates (i.e. both ground and excited states) of the quantum Heisenberg model (which has off-diagonal matrix elements in contrast to the Ising (diagonal) model).

In §2 we explain the model in detail together with some technical specifications to numerically diagonalize the Hamiltonian. Main results are presented in §3 on the ground state energy and order parameters. Discussions are given in §4.

§2. Model

The model Hamiltonian of the spin-1/2 Heisenberg model with random infinite range interactions is

$$H=-2\sum_{i<j}^{N} J_{ij}\boldsymbol{S}_i\cdot\boldsymbol{S}_j. \tag{1}$$

The exchange interaction J_{ij} obeys the distribution

$$P(J_{ij})=\frac{1}{2}\,\delta(J_{ij}-J_1)+\frac{1}{2}\,\delta(J_{ij}-J_2),$$
$$J_{1,2}=\tilde{J}_0/(N-1)\pm\tilde{J}/\sqrt{N-1}, \tag{2}$$

for all pairs (i, j). The factor $N-1$ comes from the requirement that the Hamiltonian must be exactly proportional to N even for a finite size system. According to central limit theorem the above distribution in the limit $N\to\infty$ is expected to give the same values of physical quantities as the conventional Gaussian law does.[9] In practice, to accelerate convergence of configurational average, we randomly selected equal numbers of J_1- and J_2-bonds instead of literally following (2). When the total number of bonds $N(N-1)/2$ is odd, difference between the numbers of J_1- and J_2-bonds was chosen to be $+1$ or -1, the sign being random. In the thermodynamic limit this prescription gives the same answer as (2) does. Another trick we used concerning the distribution function is to add a small random number ε_{ij} to J_{ij} at each bond. This procedure has served to lift ground state degeneracy found in limited number of samples. We decided to avoid degenerate ground states because degeneracy leads to indefiniteness of the expectation value of a physical quantity; if both ϕ_1 and ϕ_2 are ground states:

$$\langle\phi|A|\phi\rangle=|c_1|^2\langle\phi_1|A|\phi_1\rangle+|c_2|^2\langle\phi_2|A|\phi_2\rangle$$
$$+2\,\mathrm{Re}\,c_1^*c_2\langle\phi_1|A|\phi_2\rangle, \tag{3}$$

where

$$|\phi\rangle=c_1|\phi_1\rangle+c_2|\phi_2\rangle,$$

is another ground state. In (3) is seen that different coefficients c_1 and c_2 give a different expectation value. The small random number ε_{ij} to add to J_{ij} was chosen so that the average was zero and the absolute value was small enough to unchange the average of physical quantities within the significant digits we pursued.

It is easy to see that taking the complete configurational average, the average over all possible sets $\{J_{ij}\}$, is a formidable task (*e.g.*, for $N=12$, the possible number of distributing equal numbers of J_1- and J_2-bonds is about 7×10^{18}.) Therefore we have averaged over limited numbers of samples. The necessary number of samples was determined so that the sampling error was less than 0.001 (physical quantities of our interest have values of order unity as will be shown). The numbers of samples thus determined ranged from 300 to 8000 mainly depending on $\tilde{J}_0/\tilde{J}$ (many samples were required for convergence near the critical point $\tilde{J}_0/\tilde{J}\sim1$).

An account of our computational techniques to diagonalize the Heisenberg Hamiltonian is found elsewhere.[10] We just mention here that, since our computer program does not use space symmetry to reduce the size of matrices, it was possible to apply it (originally written for a system on the triangular lattice) to the present problem of a random system.

§3. Ground State Energy and Order Parameters

The ground state energy of finite size systems with $\tilde{J}_0=0$ is shown in Fig. 1 as a function of the inverse of system size. We extrapolate to $N\to\infty$ to predict $E_g/N\tilde{J}=-0.48\pm0.01$. For reference, the ground state energy of the SK model (which is obtained by dropping the x and y components from (1)) is -0.38[8] in the same unit $N\tilde{J}$. For $\tilde{J}_0>0$, a large scattering of data has prevented us from extrapolating meaningfully to $N\to\infty$.

The order parameters of interest are

$$Q=2\langle\sum_{i<j}|\langle\boldsymbol{S}_i\cdot\boldsymbol{S}_j\rangle|\rangle_c/N(N-1),$$
$$M^2=2\langle\sum_{i<j}\langle\boldsymbol{S}_i\cdot\boldsymbol{S}_j\rangle\rangle_c/N(N-1), \tag{4}$$

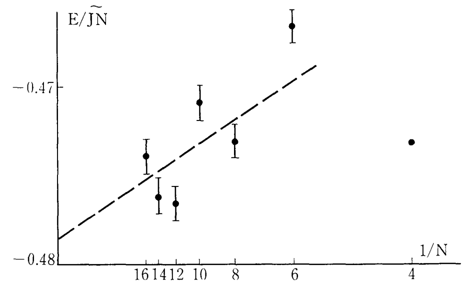

Fig. 1. The ground state energy in the case of $\tilde{J}_0=0$ is given as a function of the inverse of the system size N. Error bars represent sampling errors. By extrapolation to $N\to\infty$ we estimate $E/N\tilde{J}=-0.48\pm0.01$.

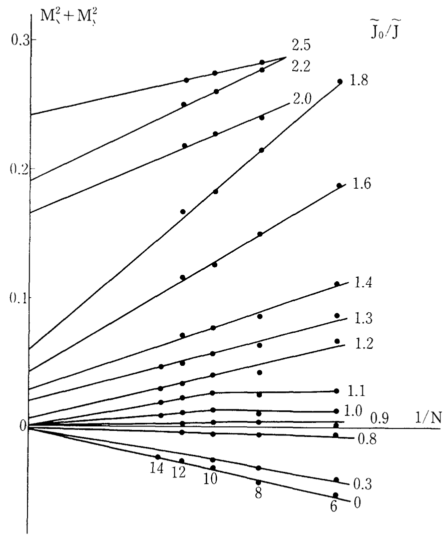

Fig. 2. The ferromagnetic order parameter M^2 is given as a function of the inverse of the system size N. Since contributions from the z-component to M^2 vanish for large enough systems in the space $S^z_{tot}=0$ (where we diagonalize the Hamiltonian), we plot M^2_{xy} obtained from (4) with $S_i \cdot S_j$ replaced by $S^x_i S^x_j + S^y_i S^y_j$. Sampling errors are smaller than the size of dots. The system size ranges from 6 to 14. The center of distribution $\tilde{J}_0/\tilde{J}$ changes from 0 to 2.5.

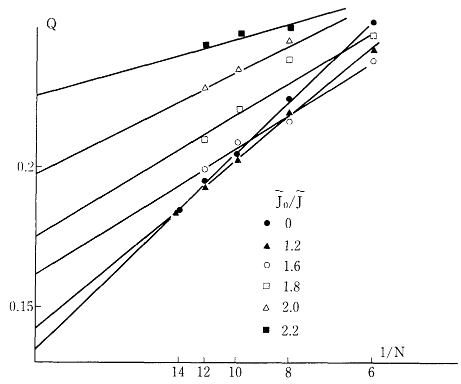

Fig. 3. The spin glass order parameter Q as a function of the inverse of the system size N. The behavior of systems with $\tilde{J}_0/\tilde{J} \lesssim 1.1$ is almost indistinguishable in the scale of this figure. Only the case $\tilde{J}_0/\tilde{J}=0$ is displayed as a representative of systems in this region.

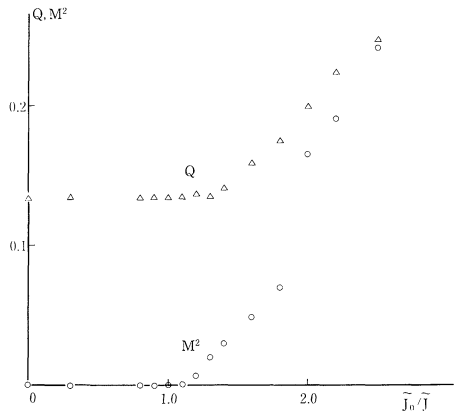

Fig. 4. Order parameters as functions of $\tilde{J}_0/\tilde{J}$. The symbol △ denotes Q and ○ is for M^2.

where the inner angular brackets denote the expectation value with respect to the ground state wave function and the outer ones $\langle \quad \rangle_c$ mean the average over the distribution of J_{ij}. Q is the spin glass order parameter and M^2 represents the conventional ferromagnetic long range order. Size dependence of these order parameters are depicted in Figs. 2 and 3. In the region $\tilde{J}_0/\tilde{J} \sim 1$, size dependence of M^2 changes between $N>10$ and $N<10$. We have discarded the data for $N<10$ in this region because the correlation length is probably large enough to exceed the system size if $N<10$, the result being the different behavior for $N<10$ and $N>10$. This observation implies a critical point at $\tilde{J}_0/\tilde{J} \sim 1$. The extrapolated order parameters shown in Fig. 4 confirm this conjecture. If $\tilde{J}_0/\tilde{J}<1$, both Q and M^2 take almost constant values, 0.135 and 0 respectively. The system is in the spin glass phase. For reference, the SK model has $Q_{SK}=0.25$ at $T=0$[3,8] (remember that our S is 1/2) although the definition of Q_{SK}[3,8] is not completely the same as ours. For $\tilde{J}_0/\tilde{J}>1$, $M^2>0$ and a ferromagnetic order develops. It is remarkable that the critical value $\tilde{J}_0/\tilde{J} \sim 1$ coincides with that of the classical Heisenberg model.[6] Therefore we conclude that quantum effects do not work in favor of either the spin glass state or the ferromagnetic phase.

In the region $1<\tilde{J}_0/\tilde{J}<2$, difference exists between Q and M^2 as observed in Fig. 4. A pure ferromagnetic ordering implies $Q=M^2$ as seen in (4). Thus the fact $Q>M^2$ means either the conventional ferrimagnetic spin ordering or that the total spin component in a certain direction does not vanish while the spin components in the perpendicular direction are randomly frozen. In the present problem it would be reasonable to assume the latter case. Hence we infer that the region $1<\tilde{J}_0/\tilde{J}<2$ corresponds to the mixed phase[6] of the classical model. For $\tilde{J}_0/\tilde{J}>2$ our data are not precise enough to determine whether $Q>M^2$ or $Q=M^2$.

§4. Discussion

Our results are summarized as follows. The ground state energy at $\tilde{J}_0=0$ is $E_g/N\tilde{J}=-0.48 \pm 0.01$, 25% lower than that of the SK model. In the region $\tilde{J}_0/\tilde{J}<1$ the system is in the spin glass phase. The order parameter Q assumes 0.135 in the whole region $0<\tilde{J}_0/\tilde{J}<1$. A phase transition has been found at $\tilde{J}_0/\tilde{J}\sim 1$, beyond which a ferromagnetic order develops. In the ferromagnetic phase $\tilde{J}_0/\tilde{J}>1$ the fact $Q>M^2$ suggests a random freezing of transverse spin components coexisting with the longitudinal ferromagnetic ordering.

As long as we characterize the system by the order parameters Q and M^2, no remarkable trace of quantum effects is found in the ground state of the Hamiltonian (1). Even the critical value $\tilde{J}_0/\tilde{J}\sim 1$ agrees with the classical prediction. Since the ground state is expected to reflect quantum effects most seriously, we may conclude that spin glasses are insensitive to quantum fluctuations in the model with infinite range interactions.

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