Two-Dimensional Randomly Frustrated Spin-1/2 Heisenberg Model

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We investigate the properties of $S = 1/2$ Heisenberg clusters with random frustration using exact diagonalizations. This is a model for a quantum spin glass. We show that the average ground state spin is $S \propto \sqrt{N}$, where N is the number of sites. We also calculate the magnetic susceptibility and the spin stiffness and low-energy excitations and discuss these in terms of a semiclassical picture.

Frustrated quantum spin systems continue to attract much interest. Such systems show rich and complex behavior, including complex ground states, with or without long-range magnetic order, quantum phase transitions at $T = 0$, and novel excitations/quasiparticles. Most work has focused on model systems with translation symmetry, in which the frustration is geometric in origin, resulting from competing antiferromagnetic exchange interactions. Typical examples are the triangular lattice [1,2] and the J_1-J_2 model on the square lattice [3–5]. We refer to such systems as "regularly frustrated." A recent review of phase transitions in frustrated antiferromagnets [6] discusses many of these issues, particularly for 3D systems. A general field theoretic approach is discussed in a recent book [7].

In contrast to these cases are systems where defects and/or random interactions or fields lead to frustration. Doty and Fisher [8] investigated the effects of both random fields and random exchange in the spin-1/2 XXZ chain and found a quantum phase transition controlled by exchange anisotropy. Sandvik [9] considered a square-lattice antiferromagnet with up to 10% ferromagnetic bonds but was unable to reach the interesting spin-glass regime. There have also been a number of studies of randomly diluted systems, but since these are not, in general, frustrated we do not discuss them further.

The most extreme case of frustration by exchange disorder occurs in spin-glass systems [10]. There is an enormous body of theoretical work on models of spin glasses, but the bulk of this is on Ising or classical XY and Heisenberg models. The earliest work on quantum spin glasses, an attempt to apply replica theory to the spin-S quantum model with long-ranged Gaussian interactions, is due to Bray and Moore [11]. The same model has been considered more recently via an SU(N) generalization [12], but the relationship of these studies to the more realistic short-range interaction case remains unclear. To our knowledge the only study of a finite S short-range spin-glass model is the work of Nonomura and Ozeki [13], who carried out exact diagonalizations on small clusters.

The present Letter is strongly motivated by Ref. [13] and extends that work in several ways. We consider small clusters of $S = 1/2$ spins with Hamiltonian

$$H = \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

where J_{ij} are random exchange interactions. Two models for randomness are used: the $\pm J$ model with

$$P(J) = \tfrac{1}{2}\delta(J - 1) + \tfrac{1}{2}\delta(J + 1), \tag{2}$$

and the Gaussian model with

$$P(J) = \frac{1}{\sqrt{2\pi}} e^{-J^2/2}. \tag{3}$$

with mean 0 and standard deviation 1. We use exact diagonalizations for clusters of $N = 10, 16, 18, 20$ spins with periodic boundary conditions. These clusters have the symmetry of the square lattice, and hence the results can be extrapolated, using finite size scaling, to the infinite lattice. We have also carried out some calculations with free boundaries, in which case our results may be relevant to magnetic nanoparticles.

The first question to be addressed is the average spin of the ground state. Using at least 500 different randomly selected bond configurations for each cluster size, we determine the ground state spin quantum number S for each realization, and the mean value and standard deviation. Of course, for the homogeneous antiferromagnet $S = 0$ rigorously, but for random interactions we find S values from 0 to 6 (for the larger clusters). Figure 1 shows histograms for $N = 18$ (periodic boundary conditions and 2000 samples) for both the $\pm J$ and Gaussian cases, together with the distribution which would be expected in the absence of interactions (the number of combinations by which one can add 18 spins 1/2 to get the total spin S). The histogram for the Gaussian model is slightly shifted to larger S compared to that for the $\pm J$ model, and the pure statistical distribution is shifted further up. However, all in all the distributions are very similar.

From the statistics of ground state spin quantum numbers we have computed the average value of S^2. One can say that this is an average value of the maximum z projection of the spin squared. This quantity has a more straightforward semiclassical meaning than $\overline{\langle S^2 \rangle} = \overline{S(S + 1)}$. In the thermodynamic limit $N \to \infty$ these two quantities coincide. The value of $\overline{S^2}$ is plotted in Fig. 2 versus N,
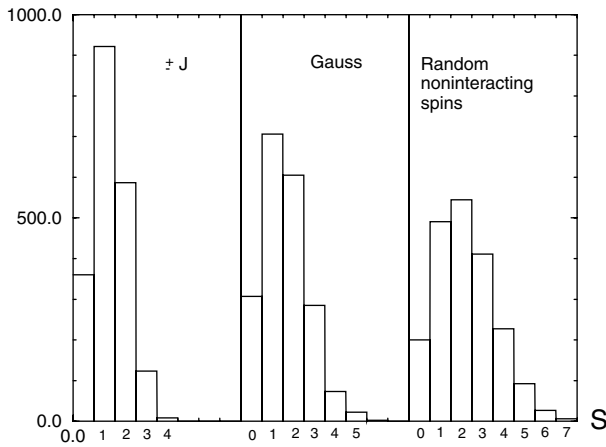
FIG. 1. The ground state spin distributions ($N = 18$ and 2000 samples) for both the $\pm J$ and Gaussian models, together with the distribution which would be expected in the absence of interactions.

the number of spins in the cluster. While there is some scatter, due both to limited statistics and to the different orientations of clusters, the data are consistent with a linear dependence of $\overline{S^2}$ on N shown by the dashed lines. In particular,

$$\pm J \text{ model:} \quad \overline{S^2} \approx 0.120N \,,$$
$$\text{Gaussian model:} \quad \overline{S^2} \approx 0.202N \,. \tag{4}$$

This means that the average spin per site varies as $1/\sqrt{N}$ and vanishes in the thermodynamic limit. This N dependence is exactly what would be expected from classical fluctuation theory, for a system of spins with random orientations, though our system is in the extreme quantum limit. If we denote the length of the effective classical spin by S_{eff}, then $\langle S^2 \rangle = N S_{\text{eff}}^2$. This yields $S_{\text{eff}} = 0.35$ for the $\pm J$ case and 0.45 for the Gaussian case, compared
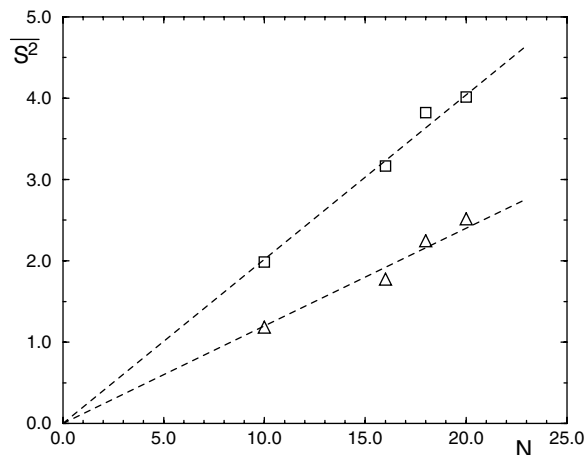

FIG. 2. The average ground state spin squared versus size of the cluster. The triangles correspond to the $\pm J$ model, and the squares correspond to the Gaussian model.

to $1/2$ for noninteracting classical spins. The quantity is reduced due to quantum fluctuations, and we observe that quantum fluctuations are greater in the $\pm J$ model than in the Gaussian case.

From the same calculations we obtain the ground state energy per spin E_0/N, averaged over at least 500 independent configurations. These values are given in Table I. There is little variation between different clusters, indicating that these results are close to the thermodynamic limit. As expected, the Gaussian model yields slightly higher energies.

We have also computed the average spin-glass order parameter in the ground state $m_{\text{sg}}^2 = \frac{1}{N^2} \overline{\sum_{i,j} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle^2}$, where the line denotes a configurational average. The values of this quantity, averaged over 500 random bond configurations, are given in Table I. Plotting the results versus $1/N$ shows a linear variation, which, when extrapolated to the bulk limit, yields $m_{\text{sg}}^2 = 0.01$ for both $\pm J$ and Gaussian cases. This value agrees with the estimate in Ref. [13]. The effective spin length S_{eff} can be estimated from the spin-glass order parameter, via $m_{\text{sg}}^2 = S_{\text{eff}}^4 \langle \cos^2 \theta \rangle = S_{\text{eff}}^4/3$, which gives $S_{\text{eff}} = 0.42$, consistent with the estimate above.

As well as the ground state we have studied properties of the low-lying excitations of the finite clusters. We have determined numerically the spin quantum number of the lowest excited state and the energy gap for at least 500 realizations of bond configurations for $N = 10, 16, 18,$ and 20 as before. We observe that predominantly (typically 97% of cases) the spin of the first excitation is $S_1 = S_0 \pm 1$, where S_0 is the spin of the ground state. In Table I we present f_+ and f_-: the fraction of configurations which have $S_1 = S_0 + 1$ and which have $S_1 = S_0 - 1$, for both $\pm J$ and Gaussian models. We also give the average energy gap $\overline{\Delta E}$ for both models, for those cases where $S_1 = S_0 \pm 1$. The average gap for $S_1 = S_0 + 1$ is practically the

TABLE I. The data for different cluster sizes N and for two types of random distribution. E_0/N is the average ground state energy per site; m_{sg}^2 is the spin glass order parameter; f_{+1} is the fraction of configurations which have spin of the first excitation $S_0 + 1$, where S_0 is spin of the ground state; f_{-1} is the fraction of configurations which have spin of the first excitation $S_0 - 1$; $\overline{\Delta E}$ is the average energy gap.

		N 10	16	18	20
$\pm J$	E_0/N	-0.493	-0.498	-0.500	-0.500
model	m_{sg}^2	0.051	0.0355	0.0325	0.0303
	f_+	0.552	0.528	0.504	0.564
	f_-	0.422	0.454	0.464	0.418
	$\overline{\Delta E}$	0.234	0.125	0.100	0.091
Gaussian	E_0/N	-0.467	-0.471	-0.472	-0.473
model	m_{sg}^2	0.050	0.0358	0.0332	0.0306
	f_+	0.512	0.484	0.466	0.510
	f_-	0.474	0.504	0.512	0.462
	$\overline{\Delta E}$	0.179	0.078	0.067	0.057

same as that for $S_1 = S_0 - 1$. The frequency f_- appears systematically less than f_+. We give an explanation of this below.

The results for the lowest excitations can be understood within a semiclassical picture, valid for large N. We denote by E_0 and $|0\rangle$ the energy of the ground state, which has total spin $S_0 \propto \sqrt{N}$, and the corresponding wave function with maximum $S_z = S_0$. We now consider an external magnetic field B in the z direction. The system will adopt a new ground state, with energy

$$E_B = E_0 - S_0 B - \tfrac{1}{2}\chi N B^2, \tag{5}$$

where χ is the magnetic susceptibility per site. The state $|0\rangle$, which will precess about the z axis with Larmor frequency $\omega = B$, is a "rigid body" excitation in which the spins precess coherently. Hence its energy with respect to E_B is simply $\delta E = S_0 B + \tfrac{1}{2}I\omega^2$. Comparing this with (5) gives the effective moment of inertia $I = N\chi$. Similar considerations can be also applied to the 2D quantum antiferromagnet and lead to the known results [14].

The lowest excitations thus correspond to the states of a 2D quantum rotor with energies

$$E_L - E_0 = \frac{L^2}{2I} = \frac{L^2}{2N\chi}, \tag{6}$$

where $L = 0, \pm 1, \pm 2, \ldots$ is the angular momentum. The total spin of the corresponding excited state is $S = S_0 + L$. Thus the lowest excitations will have $S_1 = S_0 \pm 1$, as observed in the numerical results. Note that Eq. (6) describes rotations around the z axis. This is why it is different from that for the antiferromagnet [14] which describes 3D rotations. In addition to the requirement $N \gg 1$ for this approach, we also require $|L| \ll S_0 \sim \sqrt{N}$ to justify the formula (6). In our numerical calculations this inequality is only weakly satisfied, and we believe this is the reason for the number of samples with $S_1 = S_0 - 1$ being somewhat less than with $S_1 = S_0 + 1$.

In the above consideration the susceptibility χ corresponds to the magnetic field directed along the total cluster spin. We argue that the susceptibility determined in this way from the cluster data extrapolates, in the thermodynamic limit, to the total susceptibility and not to $\chi_\perp$ (as in the antiferromagnet). This is because, in the $N \to \infty$ limit, the B^2 term in (5) will be dominant, and the energy will be independent of the spin direction.

From (6) we also see that the energy gap should behave like $1/N$. In Fig. 3 we plot the quantity $1/2\chi = N\overline{\Delta E}$ versus $1/N$. Although finite size corrections appear to be large, a rough extrapolation to $N = \infty$ gives for the magnetic susceptibility $\chi \approx 0.40$ (($\pm J$ model), and $\chi \approx 0.91$ (Gaussian). These values are about an order of magnitude higher than for the 2D quantum $S = 1/2$ antiferromagnet. Another interesting point is that the finite size correction is of the opposite sign compared to that for the 2D quantum antiferromagnet.
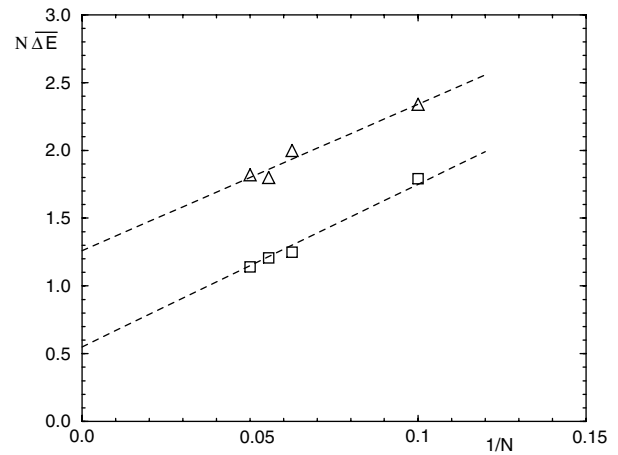

FIG. 3. The average gap $\overline{\Delta E}$ multiplied by the size of the cluster versus inverse size of the cluster. The triangles correspond to the $\pm J$ model, and the squares correspond to the Gaussian model.

The final quantity we have computed is the spin stiffness ρ_s, which is a measure of the rigidity of the ground state to a small twist θ,

$$\delta E_0 = \frac{1}{2}\rho_s \int (\nabla\theta)^2 d^2 r, \tag{7}$$

where E_0 is the ground state energy. Nonzero spin stiffness, in the thermodynamic limit, indicates a long-range magnetic order in the system. Previous calculations of ρ_s for finite antiferromagnetic clusters [15] have used a modified Hamiltonian in which the quantization axis in the twist direction is rotated by $\Delta\theta$ for neighboring sites, leading to phase factors in the exchange constants. This method of calculation assumes that the system has an intrinsic spatial periodicity, so it is applicable to ferromagnetic or antiferromagnetic states. However, we found that it cannot be applied to a random system. This is why we use a different approach. As the exact diagonalization method yields not only the ground state energy but also the ground state wave function Ψ for each cluster, we impose the twist directly on the wave function, $\Psi_\theta = U_\theta\Psi$, where U_θ is the unitary transformation which rotates each subsequent spin along a given direction by an additional angle $\Delta\theta$. The change of the energy under the twist, $\delta E_0 = \langle\Psi_\theta|H|\Psi_\theta\rangle - E_0$ is calculated explicitly, and comparison with (7) gives the spin stiffness. To avoid ambiguity we have chosen clusters with free boundaries and with the twist imposed along the x direction. Table II presents values of ρ_s for various clusters, averaged over 500 bond configurations. There is a weak decrease of ρ_s with size of the cluster, but the scatter due to different shapes does not allow us to make a reliable extrapolation. Therefore we take an average over the cluster's value as an estimate for the stiffness. We have also performed similar calculations for antiferromagnetic clusters and find that the data are very similar: a small scattering and a weak decrease with size. However, in this case we know the thermodynamic value and hence find

TABLE II. The average spin stiffness ρ_s for different rectangular clusters. The twist is imposed along the x direction.

$L_x \times L_y$	4×3	6×3	3×4	4×4	5×4
$\pm J$ model	0.220	0.208	0.214	0.200	0.198
Gaussian model	0.194	0.190	0.190	0.189	0.190

that our cluster calculations overestimate the stiffness by the factor of 1.4. Assuming that the finite size scaling factor for the random system is the same we come to the following estimates for the stiffness: $\rho_s \approx 0.15$ ($\pm J$ model) and $\rho_s \approx 0.14$ (Gaussian model). These values are just slightly less than the spin stiffness for the 2D quantum antiferromagnet on the square lattice.

Having the spin stiffness and the magnetic susceptibility we find the velocity of the Goldstone spin wave $c = \sqrt{\rho_s/\chi}$ (see Refs. [10,16]), $c \approx 0.6$ ($\pm J$ model), and $c \approx 0.4$ (Gaussian model). This should be compared with $c = 1.67$ for the 2D quantum antiferromagnet on the square lattice. The low temperature specific heat will be due to the Goldstone spin waves and thus will have a T^2 temperature dependence. We propose that this will be generic for disordered isotropic 2D quantum spin systems and explains, for example, the data for the $S = 3/2$ Kagome spin glass [17]. This should be contrasted with Ising spin glasses where the specific heat is due to the localized excitations and is linear in T.

In summary, we have investigated aspects of highly disordered $S = 1/2$ quantum spin systems at zero temperature by means of exact diagonalizations of small clusters of up to 20 spins. Averaging over disorder, we find (i) the total spin quantum number scales as $S \propto \sqrt{N}$, (ii) there is evidence of spin-glass order in the ground state, in the thermodynamic limit, (iii) the lowest excitations and energy gap for clusters are consistent with the predictions of a semiclassical theory, and (iv) the spin stiffness does not appear to scale to zero in the thermodynamic limit. Two models for the random exchange have been used, a $\pm J$ model and one with Gaussian exchange. There appears to be no significant qualitative difference between these two cases. Although we have used square lattice clusters with nearest-neighbor interactions and with periodic boundary conditions, to model the behavior of an infinite square lattice, we believe our results are more general. Although our results are obtained for rather small clusters, finite size effects appear to scale regularly and allow extrapolation to the bulk limit with reasonable confidence.

There are two ways in which our results could be related to real systems. The first is to quantum spin glasses, which have received little attention in the literature. However, one needs to be cautious in extrapolating from small clusters to systems as complex as spin glasses. An alternative application might be to disordered magnetic nanoparticles. We know of no immediate candidates. However, recent work on Mn_{12} and $Fe_{13}O_3$ spin clusters [18] (which are not disordered) suggests that this is not impossible.

Finally we remark on a recent study of a system of N randomly interacting fermions [19], in which the authors argue that ground states with zero and maximum spin will dominate. The evidence from our work is that this effect does not occur in spin clusters.

Note added in proofs.—A recent Letter by Arrachea and Rozenberg [20], which appeared after the submission of our Letter, addresses similar issues. In particular, they also observe that $\langle S \rangle \propto \sqrt{N}$.

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