Ground-state disorder in the spin-$\frac{1}{2}$ *kagomé* Heisenberg antiferromagnet

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We search for broken symmetry in the ground state of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on a *kagomé* lattice. Specifically, we calculate magnetic, spin-Peierls, spin-nematic, and chiral correlation functions in the ground states of clusters of 9, 12, 15, and 18 sites. All four correlation functions fall rapidly with distance. An analysis of their system-size dependence suggests that the ground state of this model is probably a spin liquid with the full symmetry of the Hamiltonian.

A particularly interesting consequence of zero-point fluctuations in quantum antiferromagnets is the possibility of non-Néel ground states, in which the average magnetic moment vanishes at every site.[1] These states are favored by small spin S, low dimensionality, and frustration. While they are ubiquitous in one-dimensional Heisenberg systems (given short-range interactions), their existence is much more restricted in two dimensions. In this paper we study spin correlations in one of the simplest two-dimensional models likely to support a non-Néel ground state: the antiferromagnetic Heisenberg model on a *kagomé* lattice.

This model has been suggested as a representation of two physical systems: ^{3}He adsorbed on graphite (with $S=1/2$),[2] and the layered magnetic insulator, $SrCr_{8-x}Ga_{4+x}O_{19}$ (with $S=3/2$).[3] Experiments on the latter, in particular, have stimulated a considerable theoretical effort.[4] Although the contributions of interlayer coupling and disorder to the observed magnetic properties of $SrCr_{8-x}Ga_{4+x}O_{19}$ have yet to be established, a consensus is emerging on the behavior of the *kagomé* antiferromagnet for large S. The classical ground state is highly degenerate, but small fluctuations (quantum or thermal) induce "order from disorder",[5] selecting configurations in which all spins are coplanar (spin-nematic order). Within this set of configurations there is probably also further selection, leading to three-sublattice, $\sqrt{3}\times\sqrt{3}$ magnetic order in the zero-temperature limit.[4] By contrast, for small S, rather little is known, although there is good evidence from numerical diagonalization[6] and series expansion[7] that large amplitude quantum fluctuations destroy ground-state Néel order if $S=1/2$.

There are many alternatives for the resulting non-Néel state. These include: a spin liquid which retains the full symmetry of the Hamiltonian;[1] spin-nematic[8,9] and chiral spin states,[10] with order parameters built from several spin operators; and spin-Peierls states,[11] with a broken spatial symmetry. The existence of each of these has been demonstrated in suitably designed spin models,[8,10,11] while competition between the Néel state and the magnetically disordered states has been examined in large-N generalizations of spin systems.[12]

A much studied testing ground for these ideas has been the $S=1/2$ Heisenberg model on a square lattice, with frustration introduced via second neighbor interactions (the J_1-J_2 model). One expects (from $1/S$ expansion[13]) and indeed finds (from diagonalization of small clusters and from series expansions[14]) Néel order at both small and large values of J_2/J_1, the ratio of the two exchange constants. In an intermediate regime, close to the classical degeneracy point ($J_2/J_1=1/2$), there is a magnetically disordered phase with short-range, and probably also long-range columnar dimer order,[14] as predicted by large-N theories.[12]

On the *kagomé* lattice, one can promote a disordered phase simply by reducing the spin, without tuning interactions. Different large-N theories make conflicting predictions about which non-Néel phase should then be expected. Marston and Zeng,[17] using SU(N) fermions, suggest either spin-Peierls or chiral spin states, while Sachdev,[15] using Sp(N) bosons, finds a spin liquid with unbroken symmetry. Previous diagonalization[6,16] and series expansion[7] studies of the $S=1/2$ *kagomé* model do not help in distinguishing between these possibilities, since only the magnetic correlation function[6,7] and low-lying excitation energies[6,16] have been examined.

In the following, we present results for *kagomé* lattice ground-state correlation functions, calculated on a sequence of cluster sizes. The model is defined by the Hamiltonian

$$H=\sum_{\langle i,j\rangle}\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j\ ,$$

where the sum is over all nearest neighbor pairs of sites i,j, and $\boldsymbol{\sigma}_i$ are the Pauli spin matrices. We study clusters of 9, 12, 15, and 18 sites with periodic boundary conditions, choosing the same shapes as were used by Zeng and Elser,[6] for ease of comparison with their results. For each cluster, we calculate all ground-state wave functions, $\{|G\rangle\}$, using an iterative power method. As a check on our calculation, we note that our ground-state energies coincide with those found by Zeng and Elser,[6] and by Wan;[16] we also obtain the same ground-state degeneracies as Wan.[16]

We calculate magnetic, spin-Peierls, spin-nematic, and chiral correlation functions in each ground state. These test for the most obvious, and most discussed, possible broken symmetries. Further, in a spin-$\frac{1}{2}$ system, the number of independent correlation functions that are invariant under global spin rotations is rather limited. Our choice consists of the only site-site correlation function, the only two distinct bond-bond correlation functions, and one particular triangle-triangle correlation function. In each case, we study the connected part of the correlation function, by subtracting an appropriate constant, chosen so that correlations fall to zero at long distance in the absence of broken symmetry. Specifically, the magnetic correlation between sites i and j is

$$C_M(i,j)=\langle \sigma_i \cdot \sigma_j \rangle \ .$$

The spin-Peierls correlation, written in terms of the scalar bond operator, $S_a=\sigma_1\cdot\sigma_2$ (where bond a joins sites 1

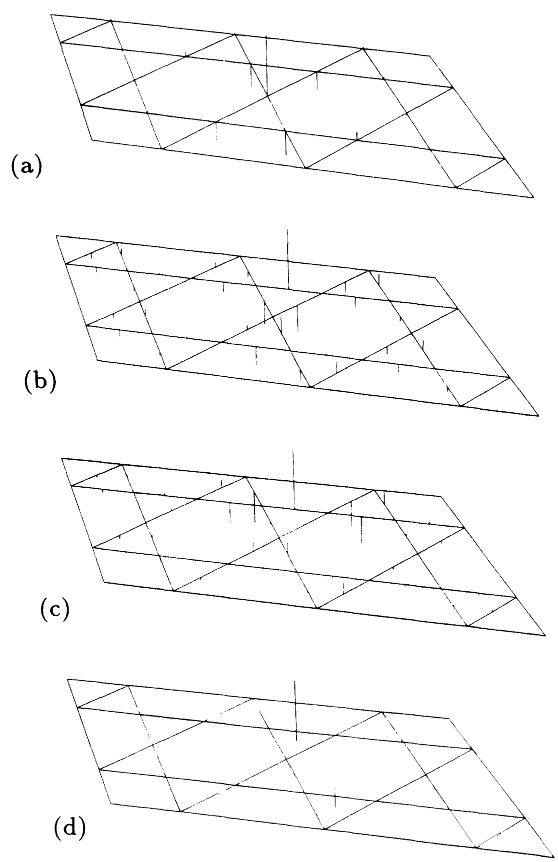

FIG. 1. Correlation functions on the 18-site cluster. Vertical lines starting at each site, bond or triangle have a length proportional to the magnitude of the correlation function at that point, and are directed up or down according to the sign. The origin in each case is the point at which the correlation function is largest. The correlation functions are (a) $C_M(r)$, (b) $C_S(r)$, (c) $C_N(r)$, and (d) $C_\chi(r)$.

TABLE I. Values of magnetic, spin-Peierls, nematic, and chiral correlation functions vs separation, r, in the 18-site cluster.

r	$C_M(r)$	$C_S(r)$	$C_N(r)$	$C_\chi(r)$
0	3.00	3.80	53.39	11.37
1	−0.80	−0.84	−7.90	−0.45
2	0.09	0.05	0.94	0.00
3	−0.03	−0.34	−1.23	−0.11

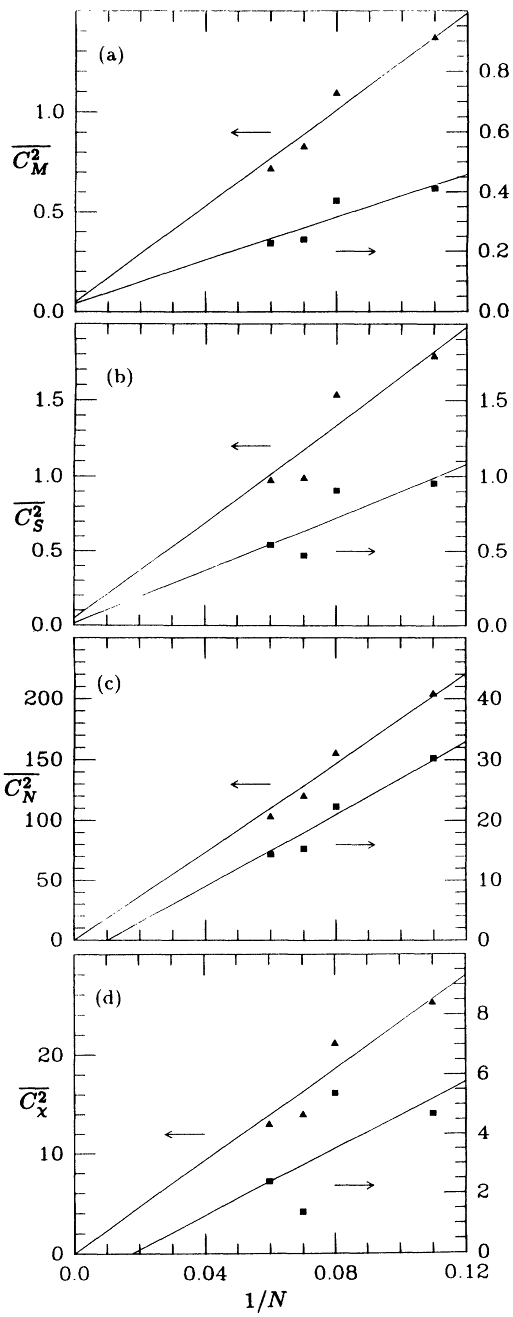

FIG. 2. Mean square of correlation functions vs inverse cluster size, $1/N$: (a) $\overline{C_M^2}$, (b) $\overline{C_S^2}$, (c) $\overline{C_N^2}$, and (d) $\overline{C_\chi^2}$. Left (right) ordinate: including (omitting) value of correlation function at zero separation in calculation of $\overline{C^2}$.

and 2), is

$$C_S(a,b)=\langle \tfrac{1}{2}(S_aS_b+S_bS_a)\rangle-\langle S_a\rangle\langle S_b\rangle \ .$$

Similarly, the spin-nematic correlation function, $C_N(a,b)$, written in terms of the vector bond operator, $\mathbf{n}_a=\boldsymbol{\sigma}_1\times\boldsymbol{\sigma}_2$, is

$$C_N(a,b)=\langle[\tfrac{1}{2}(\mathbf{n}_a\cdot\mathbf{n}_b+\mathbf{n}_b\cdot\mathbf{n}_a)]^2\rangle - \sum_{\alpha,\beta=x,y,z}\langle n_a^\alpha n_a^\beta\rangle\langle n_b^\alpha n_b^\beta\rangle \ .$$

Finally, the chiral correlation, $C_\chi(\alpha,\beta)$, between triangles α,β involves the operator $\chi_\alpha=\boldsymbol{\sigma}_1\cdot(\boldsymbol{\sigma}_2\times\boldsymbol{\sigma}_3)$, where 1, 2, and 3 are the sites at the vertices of the triangle α taken in clockwise order. It is

$$C_\chi(\alpha,\beta)=\langle \tfrac{1}{2}(\chi_\alpha\chi_\beta+\chi_\beta\chi_\alpha)\rangle \ .$$

In these definitions, $\langle\cdots\rangle$ denotes an expectation value in the ground state, or trace over ground states if $\{|G\rangle\}$ is degenerate.

The forms of these correlation functions, evaluated on an 18-site cluster, are illustrated in Fig. 1. Magnetic correlations [Fig. 1(a)], as reported by Zeng and Elser,[6] are very small beyond second neighbor separation, which is consistent with magnetic disorder predicted from series analysis.[7] Spin-Peierls correlations [Fig. 1(b)] have rather longer range. Their structure does not correspond to the type of long-range order suggested by Marston and Zeng[17] for the infinite lattice. Instead, correlations appear to reflect the geometry of the finite cluster: the clearest pattern is an alternation of sign on the sequence of four bonds parallel to the short side of the cluster.[18] A plausible conclusion is that the infinite system is either spin-Peierls disordered or only weakly ordered. Nematic correlations [Fig. 1(c)] also suggest a disordered phase. At the maximum separation allowed by this cluster size they are small and vary in sign. At nearest neighbor distance, they are large and *negative,* in complete contrast to the *positive* local nematic correlations expected for large S,[4] which illustrates how different the $S=1/2$ ground state is from the semiclassical one. Chiral correlations [Fig. 1(d)] are particularly small: they give no grounds for expecting chiral order in the infinite system. The values of these correlation functions are listed in Table I, at separation vectors parallel to the long side of the cluster.

While the nature of correlations on an 18-site cluster points towards a disordered ground state, it is clearly useful also to estimate order parameters by analyzing finite-size effects. A difficulty arises from the fact that correlation functions vary in sign without a clear pattern. Ideally, one might examine all possible ordering wave vectors; in practice, this is precluded by the small number of wave vectors allowed in our systems, and by the fact that many are allowed only in one cluster size. Instead, we study the dependence on cluster size N of $\overline{C^2}$, the average over all separations of the square of the correlation function. If correlation functions approach their asymptotic value exponentially with increasing separation, $\overline{C^2}$ will vary as $m^4+\text{constant}\cdot N^{-1}$ for large N, where m is the corresponding order parameter. This extrapolation is illustrated in Fig. 2. Since values of $\overline{C^2}$ turn out to be dominated by the rather large values of each correlation function at zero separation, we have, in addition, examined the effect of omitting these terms from the definition of the averages. These results are also displayed in Fig. 2.

In order to gauge the significance of the values of $\overline{C^2}$, extrapolated to $N=\infty$, it is useful to make comparisons with the values that $\overline{C^2}$ would take in various simple, ordered states. We have considered four such states. The first is a three-sublattice Néel state without quantum fluctuations. In this state, $\overline{C_M^2}=0.5$. The second is a simple spin-Peierls state, in which a fraction f of nearest neighbor bonds are exact singlets, without other spin correlations. For any dimer covering of the *kagomé* lattice, $f=1/4$;[2] in this case, $\overline{C_S^2}\simeq4.75$. One might expect the three-sublattice Néel state to be a good example of a nematically ordered state. In fact, although it has perfect nematic order at $S=\infty$, it has only very weak nematic order, $\overline{C_N^2}=1/36$, at $S=1/2$. An alternative comparison is with the ferromagnetically aligned state, in which $C_N=-16/3$ (negative because spins are colinear rather than coplanar) and $\overline{C_N^2}\simeq28.4$. Finally, a simple example of a chiral state is one in which every alternate triangle of spins is in the same eigenstate of the chiral operator, χ. In this state, $\overline{C_\chi^2}=9$. The extrapolated values of $\overline{C^2}$ shown in Fig. 2 are clearly much smaller than the values in these reference states.

In conclusion, both the spatial variation of correlation functions on the largest cluster studied, and an analysis of the size-dependence of order parameters, suggest that the *kagomé* Heisenberg antiferromagnet has a ground state that is either disordered or only very weakly ordered.

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