DMRG Numerical Study of the Kagomé Antiferromagnet

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We numerically study the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model on the kagomé lattice using the density-matrix renormalization group (DMRG) method. We find that the ground state is a magnetically disordered spin liquid, characterized by an exponential decay of spin-spin correlation function in real space and a magnetic structure factor showing system-size independent peaks at commensurate antiferromagnetic wavevectors. We obtain a spin triplet excitation gap $\Delta E(S = 1) = 0.055 \pm 0.005$ by extrapolation based on the large size results, and confirm the presence of gapless singlet excitations. The physical nature of such an exotic spin liquid is also discussed.

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Novel magnetic properties and the possible existence of exotic spin liquid states in low-dimensional spin-$\frac{1}{2}$ systems have attracted intensive attention in recent years. It has been established that spins in the ground state of the two dimensional (2D) nearest-neighbor Heisenberg antiferromagnet (HAF) model

$$H = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j,$$

are still ordered on square and triangular lattice systems. However, spin liquid states are likely to be found in some geometrically more frustrated systems, like the kagomé lattice, which may be seen as a diluted triangular lattice (see Fig. 1) with larger geometrical frustration and lower coordination number than the triangular lattice. Earlier exact diagonalization (ED) studies suggest that the kagomé antiferromagnet has a short-range spin correlation and a possible finite spin gap $\sim 0.05$ when the finite-size results (up to $N = 36$ sites) are extrapolated to the thermodynamic limit. Within the spin gap, a large number of singlet excited states are also identified. Recently, algebraic vortex liquid and Dirac spin liquid with gapless Dirac fermion excitations have been also proposed. Such a Dirac spin liquid state has a reasonably good variational energy but the vanishing spin triplet gap is in contrast to the ED result. While the discrepancy may be attributed to the uncertainty of the finite size effect in the ED, alternatively a finite spin gap can be also gained in the Dirac spin liquid state via an instability towards a valence bond crystal (VBC) state with a broken translational symmetry. Earlier on, Zeng and Marston also proposed that the ground state of the kagomé HAF appears to be a VBC state with a 36-site unit cell, which is supported by the series expansions. So far the precise nature of the HAF on the kagomé lattice in the long-wavelength and low-energy regime remains unsettled.

Experimentally the newly synthesized Herbertsmithite ZnCu$_3$(OH)$_6$C$_2$ has brought tremendous excitement to this field, in which the spin-$\frac{1}{2}$ copper ions form layered kagomé lattices. The absence of the magnetic ordering has been established based on the neutron scattering measurement down to $50mK$, as compared to a relatively high Curie-Weiss temperature ($\sim 300K$). The magnetic measurements also suggest that there is no signature of a finite spin gap seen in the experiment, which seems consistent with an algebraic spin liquid, but contrary to a short-range spin liquid state with a finite triplet gap. However, possible impurity spins outside the kagomé layers, caused by substitutions of nonmagnetic Zn sites with Cu, or the presence of Dzyaloshinsky-Moriya (DM) interactions may all play an important role in order to fully understand the experimental results. While the experimental situation is still unclear, on the fundamental side, it is highly desirable to reexamine the issues regarding the nature of the ground state and low-lying excitations in a pure spin-$\frac{1}{2}$ HAF model on the kagomé lattice.

Due to the geometrical frustration of the kagomé lattice, the quantum Monte Carlo (QMC) method encounters the sign problem, whereas the ED calculation is restricted to small system size. In this Letter, we present...
a systematic numerical study by employing the DMRG method[20], with keeping a large number of basis states in the DMRG blocks. We find that the ground state is indeed a magnetically disordered state, which is characterized by an exponential decay of the equal-time spin-spin correlation function in real space. The corresponding magnetic structure factor shows small peaks at commensurate momenta, with near constant peak values insensitive to the size of the system, in sharp contrast to the structure factor of the magnetic ordered state on a triangular lattice. Furthermore, we calculate the spin triplet gap, which is extrapolated to a finite value \( \Delta E(S = 1) = 0.055 \pm 0.05 \) in the large sample size limit. In this spin liquid state, there also exist low-lying singlet excitations, with their gap approaching zero at large sample size limit. Our calculations strongly hint that the ground state may be described by a resonating valence bond (RVB) spin liquid with short-range antiferromagnetic correlations and weak bond-bond and chirality-chirality correlations without explicitly breaking translational and rotational symmetries.

We consider a kagomé lattice with finite length vectors \( N_1 \mathbf{a}_1 \) and \( N_2 \mathbf{a}_2 \) as shown in Fig. 1. Here \( \mathbf{a}_1 = (2, 0) \) and \( \mathbf{a}_2 = (1, \sqrt{3}) \) are two primitive vectors of the unit cell which includes three lattice sites on a triangle. The total number of sites is \( N = 3 \times N_1 \times N_2 \), with the number of unit cells \( N_1 \times N_2 \). We will extend the calculation from \( N = 36 \) (the maximum size for ED) to much larger sizes with different geometries, up to \( N = 3 \times 16 \times 4 \) (192 sites), using the DMRG method. To test the performance of the DMRG method in the 2D spin systems, we have compared our results with the ED up to \( N = 36 \) sites for various lattices (including triangular, square, and kagomé lattices) and obtained accurate ground state energies with errors smaller than 0.01\%. For present study, we keep up to \( m = 4096 \) states in the DMRG block for most systems with more than 24 sweeps to get a converged result, and the truncation error is of the order or less than \( 10^{-5} \). We make use of the periodic boundary condition (PBC) to reduce the finite-size effect for a more reliable extrapolation to the thermodynamic limit.

We first present the DMRG result for a system with \( N = 48 \) sites \((N_1 = N_2 = 4)\). In Fig. 2(a), we show the ground state energy \( E_0 \) as a function of \( m \) — the number of states kept in each block (the dimension of the Hilbert space = \( 4m^2 \)). The ground state energy is extrapolated to \(-20.958\) at large \( m \) limit and the estimated error at \( m = 4096 \) is about 0.16\%. Similarly, the lowest energy \( E_1 \) in the total spin \( S = 1 \) sector is also shown in Fig. 2(a). Define the spin triplet gap \( \Delta E(S = 1) \equiv E_1(S = 1) - E_0 \). As plotted in the inset of Fig. 2(a), such a spin gap starts to saturate at \( m \gg 2000 \) and approaches the value 0.145 at large \( m \). In Fig. 2(b), similar results for a larger system with \( N = 108 \) \((3 \times 12 \times 3)\) are also shown, where we find a slightly larger spin gap at 0.163 for this larger but narrow system.

A systematic size dependence of the spin gap is shown in Fig. 3. In the main panel, the spin gap \( \Delta E(S = 1) \) (solid squares) vs. \( 1/N \) is plotted with \( N = 3 \times 4 \times 3, 3 \times 6 \times 3, 3 \times 4 \times 4, 3 \times 6 \times 4, 3 \times 8 \times 4, 3 \times 6 \times 5 \) and up to \( 3 \times 6 \times 6 = 108 \), together with the results of the ED (open circles) at smaller sizes (note that \( N = 36 \) site system in the ED has a different geometry as compared to the \( N = 3 \times 4 \times 3 \) system in the present calculation). All these data follow nicely a straight line shown in Fig. 3 which allows us to extrapolate the spin gap to a finite value \( \Delta E(S = 1) = 0.055 \pm 0.005 \) in the thermodynamic limit. Note that all the data presented in the main panel are for the systems close to square-like with the aspect ratio \( \alpha = N_1/N_2 \) in the range of \( 1 \leq \alpha \leq 2 \). The corresponding ground state energies per site \( E_0 \) and the spin gaps \( \Delta E(S = 1) \) for the various system sizes at a given \( m = 4096 \) are listed in Table I. Furthermore, in the inset of Fig. 3 the spin gap vs. \( 1/N \) for 3-leg \((N = 3 \times N_1 \times 3)\) and 4-leg \((N = 3 \times N_1 \times 4)\) systems with \( N_1 = 4 \) – 12 (thus including larger \( \alpha \)'s) are also present for comparison. In general, the spin gap of the 4-leg systems is smaller than that of the 3-leg systems due to the finite-size effect, consistent with the behavior shown in the main panel for the more square-like systems.
Besides the spin triplet gap $\Delta E(S = 1)$, the lowest singlet excitation energy $\Delta E(S = 0) \equiv E_1(S = 0) - E_0$ is also shown in the main panel of Fig. 3 (solid stars), whose magnitude is much smaller than $\Delta E(S = 1)$ and approaches zero with increasing sample size. This is consistent with the ED results at smaller systems, in which a large number of singlet states below the spin gap, growing with the system size, are identified. In contrast to the finite spin triplet gap, such vanishing singlet excitation energy indicates that the low-lying singlet excitations will play a dominant role in the low-temperature thermodynamic properties like specific heat.

### TABLE I: The ground state energy per site $\epsilon_0$ and spin gap $\Delta E(S = 1)$ for the square-like kagomé lattice, obtained by the DMRG with keeping $m = 4096$ basis states in one block.

| $N$           | $\epsilon_0$ | $\Delta E(S = 1)$ |
|---------------|---------------|------------------|
| $3 \times 4 \times 3$ | -0.4308 | 0.188             |
| $3 \times 6 \times 3$ | -0.43755 | 0.164             |
| $3 \times 8 \times 3$ | -0.43867 | 0.165             |
| $3 \times 10 \times 3$ | -0.43868 | 0.163             |
| $3 \times 12 \times 3$ | -0.43865 | 0.163             |
| $3 \times 4 \times 4$ | -0.43591 | 0.140             |
| $3 \times 6 \times 4$ | -0.43564 | 0.122             |
| $3 \times 8 \times 4$ | -0.43556 | 0.112             |
| $3 \times 10 \times 4$ | -0.43552 | 0.114             |
| $3 \times 6 \times 6$ | -0.43111 | 0.105             |

To characterize the ground state, the spin-spin correlation function $\langle S^z_i S^z_j \rangle$ is presented in Fig. 4 for two systems with $N = 3 \times 10 \times 3$ and $3 \times 10 \times 4$, respectively. Here $r$ is the distance between the two sites along the $\mathbf{a}_1$ direction in units of the lattice constant and the error bar denotes the mean square deviation for all the equivalent pairs of sites. Fig. 4 shows that the results are well fitted by the straight lines representing an exponential fit: $\langle S^z_i S^z_j \rangle = A \exp(-r/\tau)$ with $\tau$ as the spin correlation length whose size is insensitive to the number of legs and is about 0.8 lattice spacing for both systems (In the left lower inset of Fig. 4(b), $\tau$ as a function of $N$ is shown for a few systems up to $N = 144$). These results clearly illustrate that the ground state is magnetically disordered with no long-range correlations. Furthermore, $\langle S^z_i S^z_j \rangle$ itself exhibits short-range antiferromagnetic oscillations commensurate with the lattice constant along the $\mathbf{a}_1$ direction as shown in the top right insets of Fig. 4. Completely similar results are found for the transverse spin-spin correlation $\langle S^x_i S^x_j \rangle$ due to the spin rotational symmetry.

To further describe the short-range magnetic correlations, we calculate the static structure factor $S^z(q) = \frac{1}{N} \sum_{ij} e^{i q \cdot (\mathbf{r}_j - \mathbf{r}_i)} \langle S^z_i S^z_j \rangle$ and present the results in Fig. 5.
The peaks appear at \( q \) reciprocal lattice. These figures show that the directions of two primitive basis vectors in the re-
dering with extremely large unit cell of 36-sites.[13, 14]

It is important to observe that the peaks remain at the same small value \( \sim 0.44 \) without changing much with increasing system size, as clearly illustrated by Fig. \( \text{c} \) for the peak values at \( q^* = (\pi, \pi) \). Such weak and size-independent peaks are in sharp contrast to the structure factor of a magnetic ordered system in the triangular HAF model as shown in Fig. \( \text{d} \) with \( N = 6 \times 6 \) sites, where sharp peaks appear at \( q^* = (\frac{2\pi}{3}, \frac{2\pi}{3}) \) and \( (\frac{4\pi}{3}, \frac{4\pi}{3}) \).

Finally, we have also checked the bond-bond and chirality-chirality correlations and found that both are short-ranged with exponential-decay behavior. Thus, there seems no explicitly broken translational or rotational symmetry to be responsible for the gapless singlet excitation found in such a system. However, for our DMRG calculation with finite system size (up to 192 sites), it is difficult to detect the possible VBC ordering with extremely large unit cell of 36-sites.[13, 14]

On the other hand, the overall features of the structure factor in Fig. \( \text{a} \) and \( \text{b} \) are quite similar to those calculated[22] based on the Gutzwiller projected Dirac spin liquid state,[11] although the spin gap vanishes in the latter. One may thus conjecture the ground state for the kagomé HAF be described by an RVB state, which is similar to the projected Dirac spin liquid state at short ranges. But at long ranges it will have a finite spin triplet gap because of the finite size of spin RVB pairing, and the gapless singlet excitations are Goldstone modes originated from the broken \( U(1) \) gauge symmetry due to the RVB condensation, like in a charge-neutral superconductor. We shall use the variational QMC method to further study such kind of spin liquid states and compare with the numerical results elsewhere.

In summary, we have numerically studied the ground state properties and low-lying excitations of the kagomé antiferromagnet using the DMRG method. Our results provide strong evidence that the ground state is a spin liquid with only short-range antiferromagnetic correlations without a magnetic order or other translational or rotational symmetry breaking. The spin triplet excitation has a gap extrapolated to a finite value in the thermodynamic limit, but the singlet excitation remains gapless. The nature of such a spin liquid state has been discussed based on the numerical results.

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For example, for $N = 3 \times 6 \times 6$, the energy $\epsilon_0 = -0.43111$ at $m = 4096$ is shown in Table I. We have also calculated $\epsilon_0$ as a function of $m$ (up to $m = 4096$), which give rise to an extrapolation of the energy $\epsilon_0 = -0.43308$ at $m \to \infty$.

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