Comment on "Kagomé Lattice Antiferromagnet Stripped to Its Basics"

In a recent Letter, Azaria *et al.* [1] studied a 3-spin wide strip of the Kagomé-lattice spin-$\frac{1}{2}$ Heisenberg model, with the goal of understanding the large number of low-lying singlet states observed in 2D Kagomé clusters [2]. Using a number of approximate field-theoretical mappings, they concluded that this system had a nondegenerate, undimerized ground state, with a gap to spin excitations, but with gapless singlet excitations. The Lieb-Schultz-Mattis theorem [3], which requires there to be at least one additional zero-energy state in the thermodynamic limit, allows this never-before-seen possibility.

A subsequent study [4], using the numerical density matrix renormalization group (DMRG) [5], verified the existence of a spin gap, but was inconclusive about the key issues of degenerate ground states and gapless singlet excitations. Here, also using DMRG, we study much larger systems to examine these issues. We find that, contrary to the results of Azaria *et al.,* the ground state of this system is spontaneously dimerized, with degenerate ground states. There is a very small spin gap in the system but also a gap to singlet excitations. Above the ground states, the gap to the singlet excitations is larger than for the triplets. These results imply that this system is more analogous to the Majumdar-Ghosh model [6], rather than to a novel spin liquid. Thus, the underlying field theory needs to be reexamined.

We studied systems up to length 1024×3, keeping up to 400 states per block, using open boundary conditions. We found that the unmodified open ends of the strip have low-lying triplet end excitations, making it difficult to observe the bulk gaps. Therefore, we terminated the ends using a 2×2 cluster of spins, as shown on the left side of Fig. 1, which served to push all end excitations above the bulk gaps. Here, all exchange couplings on the ends and in the bulk have identical values J. In Fig. 2 we show the gap to the lowest-lying state, with the modified ends, as a function of the system length. We are able to resolve a very small triplet gap of $\Delta/J = 0.0104(5)$. Details of the fit will be given elsewhere.

We find that the bulk is dimerized. In Fig. 1, we show the local bond strengths, with a clearly visible dimerization

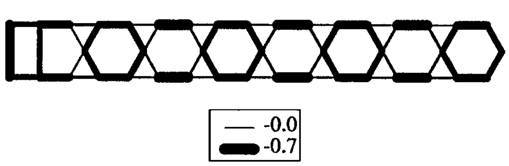

FIG. 1. The local bond strengths $\langle \vec{S}_i \cdot \vec{S}_j \rangle$ for the left end of a 32×3 strip are shown using the widths of the lines.

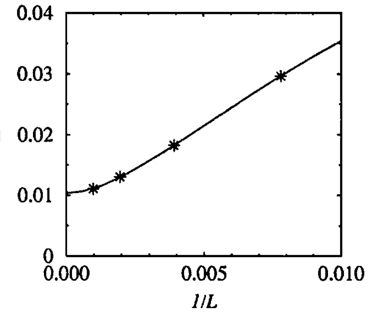

FIG. 2. Singlet-triplet gap Δ for $L \times 3$ strips as a function of the inverse length of the system.

pattern, on one end of a small 32×3 system. Results for systems as large as 1024×3 demonstrate that this dimerization pattern persists in the bulk. For example, in the bulk we find that the value of $\langle \vec{S}_i \cdot \vec{S}_j \rangle$ with i and j taking sequential values along the first leg follows the pattern -0.071, -0.529, -0.071, -0.635, -0.071, -0.529, etc. These values are well converged both in the length of the system and in the number of states kept. The singlet state representing the shifted dimerization pattern ground state is visible using periodic boundary conditions, where we found a single very low-lying singlet excited state below the triplet gap on systems as large as 48×3. In open systems, the boundaries push this state above the triplet gap. The entire pattern of states is very similar to that of the Majumdar-Ghosh model. These Kagomé strips do not provide insight into the large number of singlet states observed in 2D Kagomé clusters.

We thank Ian Affleck for discussions. This work is supported in part by the NSF under Grants No. DMR98-70930, No. PHY94-07194, and No. DMR96-16574.

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Received 3 March 2000
PACS numbers: 75.10.Jm, 75.40.Gb

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 0031-9007/00/85(15)/3330(1)$15.00