Numerical Evidences of Fractionalization in an Easy-Axis Two-Spin Heisenberg Antiferromagnet

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(Received 16 August 2004; published 15 April 2005)

Based on exact numerical calculations, we show that the generalized kagome spin model in the easy-axis limit exhibits a spin liquid, topologically degenerate ground state over a broad range of phase space, including a point at which the model is equivalent to a Heisenberg model with purely two-spin exchange interactions. We further present an explicit calculation of the gap (and dispersion) of ''vison'' excitations, and exponentially decaying spin and vison two-point correlators. These are hallmarks of deconfined, fractionalized, and gapped spinons. The nature of the phase transition from the spin-liquid state to a magnetic ordered state tuned by a negative four-spin ''potential'' term is also discussed in light of the low energy spectrum. These results greatly expand the range and the theoretical view of the spin-liquid phase in the vicinity of the Rokhsar and Kivelson exactly soluble point.

DOI: 10.1103/PhysRevLett.94.146805 PACS numbers: 73.21.–b, 11.15.–q, 73.43.Lp, 75.10.Hk

It has been demonstrated that electronic systems can have fractionally quantized excitations in nature through the discovery of the fractional quantum Hall effect (FQHE). The possibility of such fractionalization in spin systems, without any applied magnetic field, is a subject of great interest. Anderson first proposed that two-dimensional (2D) spin-$1/2$ antiferromagnets might condense into a featureless ''spin-liquid'' quantum ground state [1], with deconfined spinon excitations carrying spin $S = 1/2$ [2,3]. In the past several years, a clear notion of fractionalized and gapped [4] spin-liquid states emerged. With the absence of spin ordering and spatial symmetry breaking, such a liquid state is characterized by ''topological order'' [5,6], as in the FQHE [7]. Spinons are subject to long-range statistical interactions with vortex-like excitations (denoted as visons) which carry an Ising or Z_2 flux [8,9].

Theoretically a few spin models have been identified as possible candidates for realizing such a spin-liquid phase [10–15]. Moessner and Sondhi [12] have suggested this might occur for some antiferromagnets on the triangular lattice, by showing that a particular so-called ''quantum dimer model'' on the triangular lattice is in a featureless deconfined spin-liquid phase in a range of parameters, the lowest excitations being identified as visons [15]. Similar dimer models on the square lattice display a deconfined critical point [3] separating two confined phases. However, quantum dimer models, which have resonating valence bond correlations built in, do not derive directly from triangular or square lattice spin exchange models, so *which* spin Hamiltonian might realize this state is currently unclear.

Balents, Fisher, and Girvin [10] have recently displayed a spin model on the kagome lattice, closely mathematically related to the above triangular dimer model, which demonstrably has a fractionalized, topologically ordered ground state. Similarly to earlier studies on various dimer models [12,13], fractionalization is established through mapping the system to an exactly soluble point, first exploited by Rokhsar and Kivelson (RK) [3] in the square lattice. A drawback of this approach is that the RK point requires four-spin couplings, and topological order is argued perturbatively from the RK point. Reference [10] speculated, however, that the spin-liquid state may persist to a simpler limit describable by only two-spin Heisenberg interactions. This central issue remains unsettled.

In this Letter, we present exact numerical diagonalization studies of a generalized kagome spin model [10] in the easy-axis limit (see below) which interpolates between the RK point and a two-spin Heisenberg form—and beyond. We have found that the spin-liquid phase persists over a wide range of parameters including the two-spin limit. This phase is characterized by the absence of spin ordering, and by deconfined, fractionalized, and gapped spinon excitations. The spin-liquid phase has fourfold topological degeneracy, a finite gap to the vison excitations, and short-range exponentially decaying spin and vison two-point correlators. Still farther from the RK point beyond the two-spin model, a first order transition to a magnetically ordered phase occurs.

The model considered in most of this Letter is the generalized spin-$1/2$ ring-exchange Hamiltonian:

$$\mathcal{H} = \sum_{\bowtie}(-J_{\rm ring}S_1^+S_2^-S_3^+S_4^- + \text{H.c.} + u_4\hat{P}_{\rm flip}), \qquad (1)$$

where the labels $1, \ldots, 4$ denote the four spins at the ends of each bow tie (and others obtained by 120° rotations), as labeled in Fig. 1. The additional term is a projection operator,

$$\hat{P}_{\rm flip} = |\uparrow\downarrow\uparrow\downarrow\rangle\langle\uparrow\downarrow\uparrow\downarrow| + |\downarrow\uparrow\downarrow\uparrow\rangle\langle\downarrow\uparrow\downarrow\uparrow|, \qquad (2)$$

with spin states $S_1^z, S_2^z, S_3^z, S_4^z$ indicated sequentially in the bras/kets. This Hamiltonian acts in the reduced Hilbert space with the constraint that for each hexagon, the total S^z of six spins, $S^z_{\hexagon} = 0$. For the particular value $u_4 = 0$, Eq. (1) can be shown to be equivalent to the leading-order

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effective Hamiltonian describing the easy-axis limit of the Heisenberg model,

$$\mathcal{H} = 2\sum_{(ij),\mu} J_{ij}^{\mu} S_i^{\mu} S_j^{\mu}, \tag{3}$$

where the sum is over pairs of sites (ij), with nonzero $J_{ij}^{\mu} = J_\mu$ ($\mu = x$, y, and z) for all first, second, and third nearest-neighbor pairs (ij) on the kagome lattice (see Fig. 1). Specifically, in the extreme easy-axis limit, $J_z \gg J_\perp = J_x = J_y$, Eq. (3) reduces by second order degenerate perturbation theory to Eq. (1) with $J_{\rm ring} = 4J_\perp/J_z^2$ and $u_4 = 0$. The energy of states with $S_{\hexagon}^z \neq 0$ is higher by $O(J_z)$, and such states require additional terms beyond those in Eq. (1) for their description.

The exact soluble RK point corresponds to $u_4 = J_{\rm ring}$. For $u_4 = J_{\rm ring} - \epsilon$, with $\epsilon \ll J_{\rm ring}$, the ground state is a featureless spin-liquid state with gaps to all excitations. In particular, the vison gap was argued variationally to be $O(J_{\rm ring})$ [10]. We have performed exact Lanczos diagonalization in the whole range of $-2 \leq u_4 \leq 1$ (we take $J_{\rm ring} = 1$ as the unit). Specifically, we consider a finite-size system on the torus with length vectors $\vec{L}_1 = n_1\vec{a}_1$ and $\vec{L}_2 = n_2\vec{a}_2$, which connect identical sites [periodic boundary condition (PBC)]. Here $\vec{a}_1$ and $\vec{a}_2$ are the primitive vectors shown in Fig. 1, and we set lattice constant $a_1 = a_2 = 2$ for convenience. Then total number of sites is $N_s = 3n_1n_2$. In the constrained Hilbert space with $S_{\hexagon}^z = 0$, this problem is characterized by two topological Z_2 "winding numbers," (w_1, w_2)

$$w_a = \prod_k 2S_k^z = \pm 1, \tag{4}$$

where, for concreteness, the product is taken on one arbitrarily chosen straight line of sites along the $\vec{a}_1/\vec{a}_2$ axis for $a = 1, 2$ encircling the torus. These two winding numbers are complete in that other winding numbers defined on other nontrivial loops are not independent of these.

Shown in Fig. 2 is the excitation energy gap between the lowest two states $E_g = E(2) - E(1)$ in the topological sector with winding numbers $(1, 1)$. As u_4 moves away from 1, the energy gap remains at the order of 1 and becomes much smaller only on the negative u_4 side. All curves actually cross over each other around $U_c = -0.5$, and E_g overall decreases with the increasing of N_s with a trend of going to zero in the regime $u_4 < U_c = -0.5$. To examine the finite-size effect of transition, we show the slope of the E_g curve vs u_4 in the inset of Fig. 2 for large sizes $N_s = 42$–60. Indeed around $U_c = -0.5$, a strong peak showed up in $\Delta E_g/\Delta u_4$, with its height increasing with N_s, which is suggestive towards a quantum phase transition at U_c to a different phase with vanishing E_g.

At the RK point, a finite gap E_g is expected, related to the excitation energy of vison excitations [10], and as just discussed, this gap persists for $U_c < u_4 \leq U_{\rm RK} = 1$. Visons are characterized by the Z_2 flux $\Phi_\pi = \pm 1$, which is defined on each triangular plaquette of the kagome lattice [10] as $\Phi_\triangle = \prod_{\bowtie\in\triangle}\prod_{i\in\bowtie} 2S_i^x$, where the first product is over the three bow ties centered on the sites of the triangle, and the second is over the sites of each bow tie. It is simple to show that a ground state $|0\rangle$ of $\mathcal{H}$ can always be found which is expressed as a superposition of S_i^z eigenstates with *positive real* coefficients. This implies that $\langle 0|\Phi_\triangle|0\rangle > 0$; hence, there are no visons in the ground state. One can readily show that with PBCs the product of $\Phi_\triangle$ over all triangular plaquettes (even over just all say up-pointing triangles) is $+1$; hence visons ($\Phi_\triangle = -1$) can appear only in pairs with PBCs for $\mathcal{H}$. An appropriate definition of a single vison state is made as follows. We imagine a large open system and perform the canonical transformation

$$\mathcal{H}' = \hat{v}_{i0}\mathcal{H}\hat{v}_{i0}, \tag{5}$$

where $\hat{v}_{i0}$ denotes a single vison creation operator identified in Ref. [10], which is a "string" operator made of the product of spins $2S_i^z$ along some path on the kagome lattice starting at site i_0 and ending at the boundary. Explicitly, $\mathcal{H}'$ is the same as the $\mathcal{H}$ except that the ring-exchange terms of the three bow ties centered on the triangle containing i_0 from which the path exits are changed in sign (as

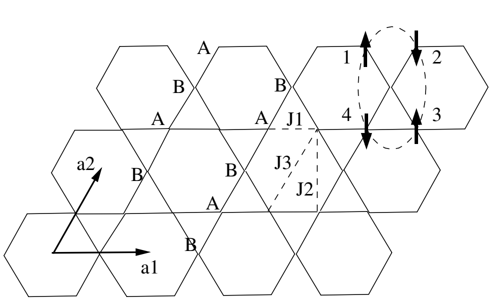

FIG. 1. Kagome lattice and interactions. Two primitive vectors $\vec{a}_1, \vec{a}_2$ are shown, as are the three two-spin couplings on sites within a hexagon. The ring term involves four sites on a bow tie, which is generated from two-spin virtual exchange processes. Sublattice labeling is also shown.

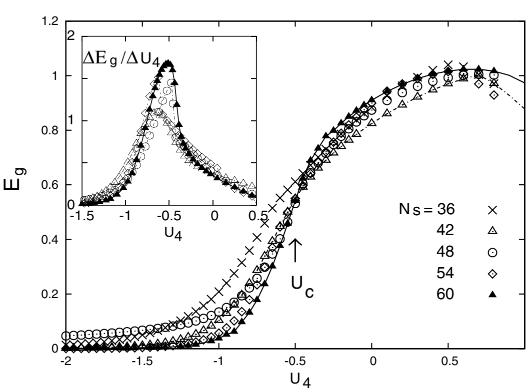

FIG. 2. The spectral gap $E_g = E(2) - E(1)$ in the winding sector $(1, 1)$ as a function of u_4 for sizes $N_s = 36$, 42, 48, 54, and 60. In the inset, $\Delta E_g/\Delta u_4$ vs u_4 for $N_s = 42$–60 (same symbols as in the main plot).

a flux tube is inserted this way). This canonical transformation *redefines* the Z_2 flux on this triangle only by a minus sign, $\Phi_\triangle \to -\Phi_\triangle$; i.e., a vison on this triangle corresponds now to $\Phi_\triangle = +1$. Imposing PBCs on $\mathcal{H}'$ (it is no longer canonically conjugate to $\mathcal{H}$) then *forces* the total number of visons to be odd. Although it is not manifest, $\mathcal{H}'$ has a hidden "magnetic" translational invariance, so there is no localization of the forced vison. Thus the energy difference between the ground states of the two Hamiltonians $E_{sv} = E'(0) - E(0)$ gives the single vison energy. We plot E_{sv} vs u_4 in Fig. 3(a) for system sizes $N_s = 36$–60.

E_{sv} shows overall similar behavior to the spectral gap E_g, but bigger than $0.5E_g$ in the vison gapped regime, indicating a nonvanishing binding energy between two visons. In the vison gapped regime, we find that the low energy manifold of $\mathcal{H}'$ forms an energy band of single visons with very small dispersion (e.g., for $N_s = 60$ dispersion of single vison energy is about $0.047J_{\text{ring}}$ at $u_4 = 0$). E_{sv} remains to almost constant in the regime passing $u_4 = 0$ and drops significantly at the $u_4 < U_c = -0.5$ side.

To reveal the nature of the phase transition at U_c, we present the low energy spectrum for $N_s = 60$ in topological sectors $(1, 1)$ and $(-1, 1)$ [states in (w_1, w_2) with $w_2 = -1$ are not shown here as they are degenerate with the ones of $w_2 = 1$ for this cluster] by plotting $\Delta E_n = E(n) - E_{\text{ground}}$ vs u_4 in Fig. 3(b) (where E_{ground} refers to the lowest state energy of the system). Clearly, in the whole range of $u_4 > U_c$, the lowest energy states from both sectors remain quasidegenerate (filled up triangle; is the energy difference). At $u_4 < U_c$, the states with different winding numbers along $\vec{L}_1$ are separated into two groups. All the low energy states from the sectors $(1, 1)$ go down and collapse with the ground state. The other $(-1, 1)$ states rise and become well separated from the low energy manifold. This dependence on the topological sector is evidence of developing spin long-range ordering. The phase transition between the vison gapped state and the spin ordered phase seems likely first order as E_g crosses at U_c and becomes zero at $u_4 < U_c$ side. Theoretically, it seems possible for such a quantum phase transition from a Z_2 spin liquid to a magnetically ordered state to be continuous [16], despite the above contrary indications. Whether our result is particular to this model or due to the reduced XY symmetry remains an open question.

The exponential decay of the vison-vison correlation function is considered as the hallmark of a 2D Z_2 fractionalized phase [8]. Following Ref. [10], we define the spin and the vison two-point correlation functions:

$$C_{ij} = 4|\langle 0|S_i^z S_j^z|0\rangle|, \qquad V_{ij} = |\langle 0|\textstyle\prod_{k=i}^{j} 2S_k^z|0\rangle|, \qquad (6)$$

where $|0\rangle$ denotes the ground state, and the product in V_{ij} is taken along some path on the kagome lattice starting at site i and ending at site j, containing an even number of sites, and making only "$\pm 60°$" turns left or right.

To examine the longer distance behavior, we considered a strip geometry with $\vec{L}_2 = 2\vec{a}_2$, while varying $\vec{L}_1 = n_1\vec{a}_1$. A similar analysis of the spectral gap E_g and single vison energy E_{sv} reveals that the critical U_c for striplike samples is slightly more negative than that for more two-dimensional clusters, around -0.75.

The numerically calculated C_{ij} is shown in Fig. 4 for $N_s = 66$ and different u_4. At $u_4 = 1$ (RK point), C_{ij} clearly shows the exponential decay seen previously from the exact wave function [10]. As u_4 varies from 1 to 0, apart from a small oscillation, we see essentially the same exponential behavior. The data at $u_4 = 1$ and 0 can both be well fitted by $\ln C_{ij} \sim -|x_i - x_j|/\xi$ with apparently the same correlation length $\xi \approx 1.7$. For u_4 further decreased to -0.4, just before the phase transition, much stronger fluctuations emerge between $x_i - x_j$ even or odd, but the overall decay remains exponential. At $u_4 = -1$, C_{ij} jumps by more than 1 order of magnitude at a longer distance $x_i - x_j = L_1/2 = 11$, and a longer range correlation is clearly evident.

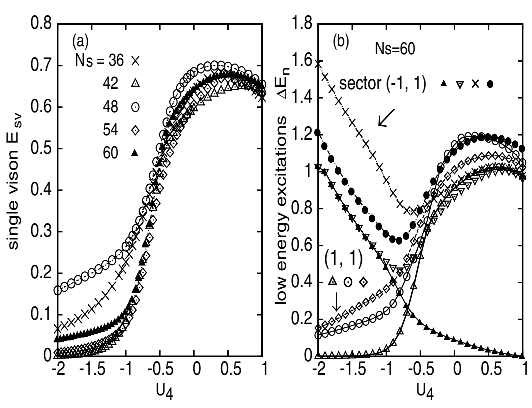

FIG. 3. (a) The single vison energy $E_{sv} = E'(0) - E(0)$ as a function of u_4 for system sizes $N_s = 36$, 42, 48, 54, and 60; (b) the low energy spectrum $\Delta E_n = E(n) - E_{\text{ground}}$ for $N_s = 60$ ($L_1 = 5a_1$ and $L_2 = 4a_2$), in topological sectors $(\pm 1, 1)$ vs u_4.

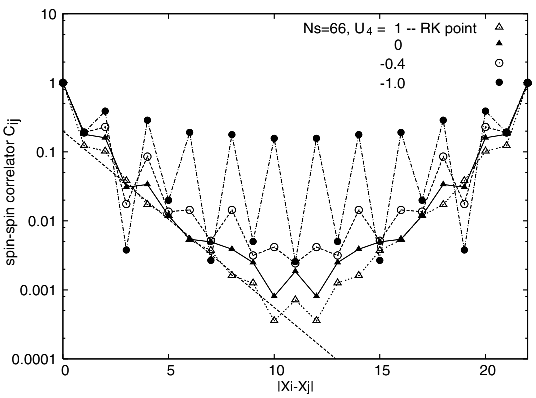

FIG. 4. The spin correlator C_{ij} vs distance $x_i - x_j$ at $u_4 = 1, 0, -0.4$, and -1 for a striplike system at $N_s = 66$.

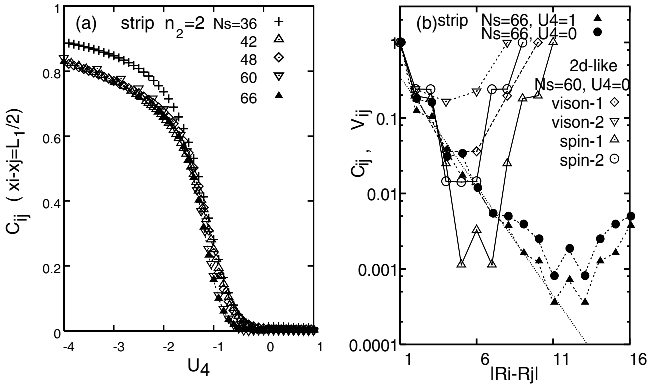

FIG. 5. (a) C_{ij} at fixed $x_i - x_j = L_1/2$ vs u_4 for a striplike system at $N_s = 36$, 42, 48, 60, and 66. (b) Vison correlator V_{ij} along $\vec{a}_1$ (vison 1) and $\vec{a}_2$ (vison 2) for the 2D-like system $N_s = 60$ are compared with C_{ij} for both the 2D system at $N_s = 60$ and the strip system at $N_s = 66$.

We analyze the finite-size dependence of the spin correlation function. In Fig. 5(a), C_{ij} with $j = i + L_1/2$ (halfway across the torus) is shown for relatively large sizes $N_s = 36$, 42, 48, 54, 60, and 66. For $u_4 > U_c$ (around -0.75), C_{ij} is vanishingly small for all sizes. For $u_4 < U_c$, however, C_{ij} is very weakly dependent on N_s (except for the smallest system with $N_s = 36$), and it robustly scales to a finite value at large N_s limit. This strongly indicates long-range magnetic order. One expects this region is adiabatically connected to the $u_4 \to -\infty$ limit, for which the ground state is fully magnetically ordered state with $4\langle S_i S_j \rangle = \pm 1$, taking the positive or negative sign if i and j belong to the same or different sublattices, respectively (see sublattices A and B labeling in Fig. 1; spins not belonging to these two sublattices are not ordered). In the strip geometry for large negative u_4, one can show the ground state manifold (with fourfold degeneracy) is well separated from excited states by an energy gap of $4J_{\rm ring}/|u_4|^2$, with additional ordering in the x-y plane (in spin space), as a result of order-by-disorder phenomena. At the critical U_c, we have also observed a very similar change in the behavior of the vison two-point correlator from exponential decay to the long-range correlation.

We further examine the vison and spin correlators in more 2D clusters. We plot C_{ij} and V_{ij} at $u_4 = 0$ for a cluster of $N_s = 60$, with $L_1 = 5a_1$ and $L_2 = 4a_2$, vs $R_i - R_j$ in Fig. 5(b). Despite the very short distance across the torus, several points indeed follow an exponential behavior comparable with C_{ij} for the strip with $N_s = 66$. Clearly, all the correlators can be well fitted by $\exp(-|R_i - R_j|/\xi)$ (as the dashed line in the plot) with $\xi \approx 1.7$.

In summary, a fractionalized spin-liquid state has been identified for the generalized kagome spin model beyond the RK exact soluble point, which persists over a wide range of parameters, covering the pure two-spin kagome Heisenberg model at easy-axis limit ($u_4 = 0$). We have also established a precise way of identifying a spin-liquid phase based on exact diagonalization (with and without inserting a flux tube), which can be applied to various spin models on other lattices. These methods can refine approximate calculations (variational and density-matrix renormalization group methods) suggesting the lack of dimer ordering, finite spin gap, and possible spin-liquid behavior in other models [17].

We acknowledge stimulating discussions with Matthew Fisher, and both stimulation and patient explanation from Arun Paramekanti. This work was supported by ACS-PRF 41752-AC10, Research Corporation Grant No. CC5643, the NSF Grants No. DMR-0307170 (D. N. S.) and No. DMR-9985255, and the Sloan and Packard Foundation (L. B.). We thank the Aspen Center for Physics and Kavli Institute for Theoretical Physics for hospitality and support (through PHY99-07949 from KITP), where part of this work was done.

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