Numerical study of fractionalization in an Easy-axis Kagome antiferromagnet

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(Dated: June 6, 2021)

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. We present an (to our knowledge the first) explicit calculation of the gap (and dispersion) of “vison” excitations, and exponentially decaying spin and vison 2-point correlators, hallmarks of deconfined, fractionalized and gapped spinons. The region of the spin liquid phase includes a point at which the model is equivalent to a Heisenberg model with purely two-spin interactions. Beyond this range, a negative “potential” term tunes a first order transition to a magnetic ordered state. The nature of the phase transition is also discussed in light of the low energy spectrum. These results greatly expand the results and range of a previous study of this model in the vicinity of an exactly soluble point\textsuperscript{a}.

PACS numbers: 73.21.-b, 11.15.-q, 73.43.Lp

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{kagome_lattice.png}
\caption{Kagome lattice and interactions. Two primitive vectors $\vec{a}_1, \vec{a}_2$ are shown, as are the three 2-spin couplings on sites within a Hexagon. The ring term involves four sites on a bow-tie, which is generated from 2-spin virtual exchange processes. Sublattice labeling is also shown.}
\end{figure}

The discovery of the fractional quantum Hall effect (FQHE) has revealed that electronic systems can have fractionally quantized excitations in nature. 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\textsuperscript{2}, with deconfined spinon excitations carrying spin $S = 1/2$. In the past several years, a clear notion of fractionalized and gapped spin-liquid states emerged. With the absence of spin ordering and spatial symmetry breaking, such a liquid state is characterized by “topological order”\textsuperscript{2}, as in the FQHE\textsuperscript{2}. Spinons are subject to long-range statistical interactions with vortex-like excitations (denoted as visons) which carry an Ising or $Z_2$ flux\textsuperscript{9,10}.

Theoretically a few spin models have been identified as possible candidates for realizing such a spin liquid phase\textsuperscript{1,11,12,13,14}. Moessner and Sondhi\textsuperscript{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. Unfortunately, the triangular quantum dimer model does not derive directly from a triangular lattice spin model, so which spin Hamiltonian might realize this state is currently unclear. Similar dimer models on the square lattice display only a deconfined critical point\textsuperscript{a}, separating two confined phases.

Balents, Fisher and Girvin\textsuperscript{2} 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\textsuperscript{12,13}, fractionalization is established through mapping the system to an exactly soluble point, first exploited by Rokhsar and Kivelson (RK)\textsuperscript{4} 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. Ref\textsuperscript{11} 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\textsuperscript{4} 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 four-fold topological degeneracy, a finite gap to the vison excitations, and short range exponentially decaying spin and vison 2-point correlators. Still further from the RK point beyond the 2-spin model, a first order transition to a magnetically ordered phase occurs.

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

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

where $S_i^\pm = S_i^x \pm i S_i^y$ and $\hat{P}_{\text{flip}}$ is the Pauli flip operator on the ring.
where the labels 1 . . . 4 denote the four spins at the ends of each bowtie (and others obtained by 120 degree rotations), as labeled in Fig. 1. The additional term is a projection operator,

\[ \hat{P}_{\text{flip}} = \vert \uparrow \downarrow \uparrow \downarrow \rangle \langle \uparrow \downarrow \uparrow \downarrow \vert + \vert \downarrow \uparrow \downarrow \uparrow \rangle \langle \downarrow \uparrow \downarrow \uparrow \vert, \]

with spin states \( S_i^l, S_i^r, S_i^z \) 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, \( S_0^z = 0 \). For the particular value \( u_4 = 0 \), Eq. (1) can be shown to be equivalent to the leading-order effective Hamiltonian describing the easy-axis limit of the Heisenberg model,

\[ \mathcal{H} = 2 \sum_{(ij), \mu} J_{ij}^\mu \sigma_i^\mu \sigma_j^\mu, \]

where the sum is over pairs of sites \((ij)\), with non-zero \( J_{ij}^\mu = J_f \) for all first, second, and third nearest-neighbor pairs \((ij)\) on the Kagome lattice (see Fig. 1). Specifically, in the extreme easy-axis limit, \( J_z \gg J_f \), Eq. (2) reduces by second order degenerate perturbation theory to Eq. (1) with \( J_{\text{ring}} = 4J_f / J_2^2 \). The energy gap \( \Delta E \) for states with \( S_0^z \neq 0 \) 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 \( u_4 = J_{\text{ring}} \). For \( u_4 = J_{\text{ring}} - \epsilon \), with \( \epsilon \ll J_{\text{ring}} \), the ground state is a featureless spin liquid state with gaps to all excitations. In particular, the vison gap was argued variationally to be \( O(J_{\text{ring}}) \). We have performed exact Lanczos diagonalization in the whole range of \(-2 \leq u_4 \leq 1\) (we take \( J_{\text{ring}} = 1 \) as the unit). Specifically, we consider a finite size system on the torus with length vectors \( \vec{a}_1 = n_1 \vec{a}_1 \) and \( \vec{a}_2 = n_2 \vec{a}_2 \), 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 \( S_0^z = 0 \), this problem is characterized by two topological \( Z_2 \) “winding numbers”, \((w_1, w_2)\)

\[ w_a = \prod_k 2S_k^z = \pm 1, \]

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 non-trivial loops are not independent of these. Using translational invariance, the Hilbert space for \( N_s = 60 \) can be reduced to a dimension (total number of configurations) around \( N_{\text{conf}} = 3618896 \) (\( N_{\text{conf}} \) varies amongst different topological sectors).

Shown in Fig. 2 is the excitation energy gap between the lowest two states \( E_2 = E(2) - E(1) \) 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 only becomes much smaller 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\( \Phi \), and as just discussed, this gap persists for \( U_c < u_4 \leq U_{\text{RK}} \). Visons are characterized by the \( Z_2 \) flux \( \Phi = \pm 1 \), which is defined on each triangular plaquette of the Kagome lattice, as

\[ \Phi_{\Delta} = \prod_{\beta \in \Delta} \prod_{\alpha \in \alpha} 2S_k^z, \]

where the first product is over the three bowties centered on the sites of the triangle, and the second is over the sites of each bowtie. It is simple to show that a ground state \( \vert 0 \rangle \) of \( \mathcal{H} \) can always be found which is expressed as a superposition of \( S_k^z \) eigenstates with positive real coefficients. This implies that \( \langle 0 \vert \Phi_{\Delta} \vert 0 \rangle > 0 \); hence, there are no visons in the ground state. One can readily show that with PBCs the product of \( \Phi_{\Delta} \) over all triangular plaquettes (even over just all say up-pointing triangles) is \( +1 \), hence visons \( \Phi_{\Delta} = -1 \) can only appear 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

\[ \mathcal{H}' = \hat{v}_{i_0} \mathcal{H} \hat{v}_{i_0}, \]

where \( \hat{v}_{i_0} \) denotes a single vison creation operator identified in Ref. 3, which is a “string” operator made of the product of \( 2S_k^z \) along some path on the Kagome lattice starting at site \( i_0 \) and ending at the boundary. Explicitly, \( \mathcal{H}' \) is the same as \( \mathcal{H} \) 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. This canonical transformation redefines the \( Z_2 \) flux on this triangle only by a minus sign, \( \Phi_\Delta \rightarrow -\Phi_\Delta \), i.e. a vison on this triangle corresponds now to \( \Phi_\Delta = +1 \). Imposing PBCs on \( H' \) (it is no longer canonically conjugate to \( H \)) then forces the total number of visons to be odd. Although it is not manifest, \( H' \) 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. 3a 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 non-vanishing binding energy between two visons. In the vison gapped regime, we find that the low energy manifold of \( H' \) forms an energy band of single visons with very small dispersion (e.g., for \( N_s = 60 \) dispersion of single vison energy is about 0.047/J_\text{ring} at \( u_4 = 0 \)). \( E_{sv} \) remains to almost constant in the regime passing \( u_4 = 0 \), and drops significantly at \( u_4 < U_c = -0.5 \) side.

To reveal the nature of the phase transition at \( U_c \), we present the low energy spectrum for \( N_s = 60 \) in all four topological sectors by plotting \( \Delta E_n = E(n) - E_\text{ground} \) vs. \( u_4 \) in Fig. 3b (where \( E_\text{ground} \) refers to the lowest state energy of the system). Clearly, in the whole range of \( u_4 > U_c \), the lowest energy states from each topological sector remain quasidegenerate (filled triangular-up, is the energy difference). At \( u_4 < U_c \), the states with different winding numbers along \( L_1 \), are separated into two groups. All the low energy states from the sectors \((1, \pm 1)\) go down and collapse with the ground state. The other \((-1, \pm 1)\) 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. Similar results are obtained for all system sizes 36 - 66. The phase transition between the vison gapped state and spin ordered phase seems likely first order as \( E_g \) crosses at \( U_c \) and becomes zero at \( u_4 < U_c \) side. At almost the same time, the ground state degeneracy of all sectors breaks down and long-range spin order develops.

As discussed in Ref. [2], exponential decay of the vison-visoron correlation function is the hallmark of a 2d \( Z_2 \) fractionalized phase. Following Ref. [2], we define the spin and the vison 2-point correlation functions:

\[
C_{ij} = \langle 0 | S^z_i S^z_j | 0 \rangle, \quad V_{ij} = \left| \langle 0 | \prod_{k=i}^{j} 2 S^z_k | 0 \rangle \right|
\]

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 “\( \pm 60^\circ \)” turns left or right. Due to the constraint \( S_0^z = 0 \), the latter product is path-independent up to an overall sign (hence the absolute value in Eq.:).

To examine the longer distance behavior, we considered a strip geometry with \( L_2 = 2a_d \), while varying \( L_1 = n_1 a_1 \). Similar analysis of the spectral gap \( E_g \) and single vison energy \( E_{sv} \) reveals that the critical \( U_c \) for strip-like 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 wavefunction. 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 one order of magnitude at longer distance \( x_i - x_j = L_1/2 = 11 \), and a longer range correlation is clearly evident.

We analyze the finite-size dependence of the spin spin...
correlation function. In Fig. 5a, $C_{ij}$ with $j = i + L_1/2$ (halfway across the torus) is shown for relatively large sizes $N_x = 36, 42, 48, 60, 66$. 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 $N_x$ (except for the smallest system with $N_x = 36$), and it robustly scales to a finite value at large $N_x$ 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 sublattice 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 4-fold degeneracy) is well separated from excited states by an energy gap of $4J_{ring}/|u_4|^2$, with additional ordering in the x-y plane (in spin space), as a result of order-by-disorder phenomena. Details will be reported elsewhere.

We further examine the vison 2-point correlator. In the strip case, the vison correlator vanishes exponentially but with an extremely short correlation length $\xi$ much smaller than the lattice constant. For more 2d clusters, the vison correlator has almost the same $\xi$ as the spin correlator. We plot $C_{ij}$ and $V_{ij}$ at $u_4 = 0$ for cluster of $N_x = 60$, with $L_1 = 5a_1$ and $L_2 = 4a_2$, vs. $R_i - R_j$ (along both $a_1$ or $a_2$ vison-1 or vison-2) in Fig. 5b. Despite the very short distance across the torus, the several points indeed follow an exponential behavior comparable with $C_{ij}$ for the strip with $N_x = 66$. Clearly, all the correlators can be well fitted by $\exp(-|R_i - R_j|/\xi)$ (as the dashed line in the plot) with $\xi \approx 1.7$.

We conclude with some discussion of related quantum phase transitions. Our numerical calculations indicate that the fractionalized spin-liquid state, previously established for the generalized Kagome spin model at the RK point, persists in a wide range of parameters, covering the pure 2-spin Kagome model ($u_4 = 0$). On the negative $u_4$ side, a first order transition to the magnetic ordered phase happens at $U_c = -0.5J_{ring}$. It seems that the easy axis spin model easily develops long-range Ising magnetic order at the confinement transition. It is possible that this ordering is an artifact of the easy-axis limit, which suppresses some fluctuations, and perhaps Kagome antiferromagnets away from easy-axis limit may develop instead a gapless spin-liquid phase, which would be extremely interesting to explore.

We would like to acknowledge stimulating discussions with Matthew Fisher, and both stimulation and patient explanation from Arun Paramekanti. This work was supported by ACS-PRF 36965-AC5 and 41752-AC10, Research Corporation Award CC5643, the NSF grants DMR-0307170 (DNS), DMR-9985255, the Sloan and Packard foundation (LB). 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.