Dynamical Signature of Symmetry Fractionalization in Frustrated Magnets

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The nontriviality of quantum spin liquids (QSLs) typically manifests in the nonlocal observables that signify their existence; however, this fact actually casts a shadow on detecting QSLs with experimentally accessible probes. Here, we provide a solution by unbiasedly demonstrating a dynamical signature of anyonic excitations and symmetry fractionalization in QSLs. Employing large-scale quantum Monte Carlo simulation and stochastic analytic continuation, we investigate the extended XXZ model on the kagome lattice, and find out that, across the phase transitions from $\mathbb{Z}_2$ QSLs to different symmetry breaking phases, spin spectral functions can reveal the presence and condensation of emergent anyonic spinon and vison excitations, in particular, the translational symmetry fractionalization of the latter, which can be served as the dynamical signature of the seemingly ephemeral QSLs in spectroscopic techniques such as inelastic neutron or resonance (inelastic) x-ray scatterings.

Introduction.—Quantum spin liquids (QSLs) [1–4] are exotic phases of matter characterized by long-range many-body entanglement and fractionalized excitations [5]. One of the defining features of QSLs is that there is no local order parameter and the nontriviality of the phase manifests in nonlocal observables. In the case of gapped QSLs, global observables such as Wilson loop operators [6,7], topological entanglement entropies [8–10], and modular transformations [11] have been exploited to characterize topological order theoretically, but none of them are directly accessible in experiments. Available to experiments are measurements of static [12] and dynamical spin correlation functions (besides thermodynamical quantities). In particular, dynamical spin structure factor (DSSF), measured by inelastic neutron scattering, probes the spectral properties of elementary magnetic excitations [13,14]. Therefore, it is an important question for understanding what kind of universal information about the underlying QSLs can be extracted from the momentum and energy resolved DSSFs.

For example, now, a continuum in DSSF is often taken as an indication of fractionalized excitations, but a simple continuum in the spin spectrum can also be caused by disorder [15]. Therefore, additional signatures in DSSF unique to a QSL are desired. On the other hand, it is also desirable to read out more information besides the existence of fractionalized excitations from DSSF. In particular, QSLs with the same type of anyon excitations can be further classified by how internal and lattice symmetries act on the anyons, known as the symmetry-enriched topological order [5,16,17]. It has been proposed that [18–20] this additional information can also be detected from DSSF. In this work, for the first time, we compute the DSSF in a frustrated spin model in an unbiased manner and observe such unique dynamical signatures in DSSF—the fractionalization of lattice symmetries—in QSL with $\mathbb{Z}_2$ topological order.

Model and method.—We consider the extended Balents-Fisher-Girvin (BFG) model on a kagome lattice, where $\mathbb{Z}_2$ QSLs are realized [10,12,21–25]. It has been extensively investigated as one of the very few models of frustrated magnets that can be simulated with unbiased quantum Monte Carlo (QMC) methods, and the defining features of QSL such as spinon and vison excitations [23,26], topological entanglement entropy [10], and fractionalized quantum critical points [24] have been revealed.

The Hamiltonian of the model is given by

$$H = -J_\pm \sum_{\langle i,j \rangle} (S_i^+ S_j^- + \text{H.c.}) + \frac{J_z}{2} \sum_O \left( \sum_{i \in O} S_i^z \right)^2 + J'_z \sum_{\langle i,j \rangle'} S_i^z S_j^z - h \sum_i S_i^z,$$

(1)
The model is highly anisotropic and frustrated, i.e., the ordering of spins on the same sublattice [21]. The Hamiltonian in Eq. (1) depicted. (b) Brillouin zone of the kagome lattice, with the reciprocal vectors \( r \). (c) \( J_z/J_z \) phase diagram of Hamiltonian in Eq. (1) at magnetization \( m_z = 0 \) [12]. Along the \( J_z/J_z \) axis, there is a transition from \( Z_2 \) QSL to ferromagnetic (FM) ordered phase; along the \( J_z/J_z \) axis, following the direction of the red arrow, there is a transition from \( Z_2 \) QSL to the ground state manifold respects the constraint \( S^z = \sum_{i \in \xi} S^z_i = 6 m_z \) for each hexagon. Violations of these constraints correspond to deconfined excitations, the spinon, whose energy gap is of the order of \( J_z \). Since a spin flip \( S^z_i \), which carries a charge of 1 under \( U(1)_{S_z} \), creates two identical hexagon excitations, each with \( S^z = 6 m_z + 1 \), each of them must carry a \( U(1)_{S_z} \) charge of 1/2 and, thus, is called a spinon. The other kind of excitation, visons, are more subtle and can be viewed as sources of \( \pi \) flux for spinons. When a spinon is transported around a vison, its wave function changes sign. Since visons do not carry any \( U(1)_{S_z} \) charge, it is natural that \( S^z \) operators can create pairs of visons. This is supported by an explicit construction of vison states at a soluble deformation of the BFG model in Ref. [22]. Because visons are created in the low-energy manifold with \( S^z = 6 m_z \), they have a much lower energy gap of the order of \( J_z/J_z \).

Therefore, to observe the spectral information of spinon and vison excitations of \( Z_2 \) QSLs, we make use of the following dynamical spin structure factors:

\[
S^\pm_{\alpha \beta}(q, \tau) = \langle S^\pm_{q,\alpha}(\tau) S^\pm_{q,\beta}(0) \rangle,
\]

\[
S^z_{\alpha \beta}(q, \tau) = \langle S^z_{q,\alpha}(\tau) S^z_{q,\beta}(0) \rangle.
\]

Here, the imaginary time \( \tau \in [0, \beta] \), and to make sure that the system is close to the QSL ground state, we choose \( \beta = 2L/J_z \) to be below the energy scale associated with the anyonic excitation gap (if \( J_z = 0.1 J \), then \( T \leq J_z/J_z \) when \( L > 5) \). \( L \) is the linear system size and the total number of sites \( N = 3 \times L^2 \). \( \alpha, \beta = 1, 2, 3 \) label the three sublattices of the kagome lattice. \( \langle \cdots \rangle \) stands for the QMC ensemble average. We have defined \( S^\pm_{q,\alpha} = \sqrt{3/N} \sum_{i=0} e^{-iq_i r_i} S^\pm_i \), where the summation over the sublattice \( \alpha \) and \( r_i \) is the spatial position of the site \( i \). \( S^z_{q,\alpha} \) is defined in the same vein.

One can obtain the real frequency DSSFs via the stochastic analytic continuation (SAC) [29–36] of the imaginary-time data. In SAC, candidate real-frequency spectra are proposed and fitted to the imaginary time data. Each candidate is then weighted by their goodness-of-fit \( \chi^2 \) as an effective energy, such that a Metropolis sampling can be defined over the proposed spectra. The final spectrum is the ensemble average of all candidates. A detailed account of SAC and its recent applications can be found in Refs. [32–37].

Figure 2 shows the obtained \( S^\pm(q, \omega) = \frac{1}{T} \sum_{\alpha} S^\pm_{\alpha \alpha}(q, \omega) \) and \( S^z(q, \omega) = \frac{1}{T} \sum_{\alpha} S^z_{\alpha \alpha}(q, \omega) \) along the high symmetry
spinon excitations have a pair gap energy scales of the spectral gap. We expect that the value of $\Delta_0$ is $1/3$, both at $m_z = 0$ with $J_\perp = 0.06$, $J'_\parallel = 0.005$, and $m_z = 0$ with $J_\perp = 0.06, J'_\parallel = 0.005$. The system size is $L = 16$. The spectra are all gapped with continua. The spectral bottom is at $\omega \sim 0.1$, this is the energy scale of a vixon-pair as discussed in the text and consistent with the vixon-pair gap $\Delta_v$ fitted in (e) and (f). $S^{zz}(\mathbf{q}, \omega)$ along the high symmetry path at $m_z = 0$ with $J_\perp = 0.06, J'_\perp = 0.005$ for $L = 18$ (c) and $m_z = 0$ with $J_\perp = 0.06, J'_\perp = 0.005$ for $L = 16$ (d). The spectra are all gapped with continua. The spectral bottom is at $\omega \sim 0.2$, consistent with the energy scale of a spinon-pair gap $\Delta_s$, obtained in (e) and (f). (e) (f) is the temperature dependence of the energy for $L = 12$ system for parameters in (a) and (c) [(b) and (d)]. The second, much lower $\exp(-\Delta_s/T)$ happens at $\Delta_s \sim 0.1$ (see Fig. 2 insets for clarity), which is apparently the vixon-pair gap, consistent with the gap in $S^{zz}(\mathbf{q}, \omega)$ in Figs. 2(a) and 2(b). Therefore, we can conclude that the vison-pair excitations are observed in the $S^{zz}(\mathbf{q}, \omega)$ spectra and the spinon-pair excitations are observed in the $S^{zz}(\mathbf{q}, \omega)$ spectra. A similar observation for the vixon excitation in the pure BFG model at $m_z = 0$ has also been shown in Ref. [26].

Symmetry fractionalization.—Once we have established the relation between DSSF and anyonic excitation gaps, now, we set out to explore the more salient yet fundamental difference between the $\mathbb{Z}_2$ QSLs at $m_z = 0$ and $0.5$, i.e., their different form of symmetry fractionalization [38–40]. In the case of $\mathbb{Z}_2$ QSLs, spinons and visons can carry a fractional crystal momentum associated with the lattice, which means that

$$T_1^{(a)}T_2^{(a)} = -T_2^{(a)}T_1^{(a)},$$

here, $a$ refers to an anyon (i.e., spinon or vixon) and $T_1^{(a)}$ denotes the local action of translation on it. Intuitively, with such fractionalization, $a$ moves on a lattice with $\pi$ flux per unit cell.

The fractional crystal momentum carried by visons is determined by the magnetization per unit cell [41]. In $\mathbb{Z}_2$ QSLs realized in the extended BFG models, the spinon carries a half-integer spin, a fractionalized quantum number [22]. At $m_z = 0$, the spin per unit cell is $1/2$, indicating that there must be an odd number of spinons therein. As a result,
moving a vison around a unit cell results in a $\pi$ Berry phase due to its mutual braiding with the spinons. In other words, the visons must carry a fractional crystal momentum, and consequently, vison translation operators anticommute at $m_z = 0$. On the other hand, at $m_z = \frac{1}{6}$, the spin per unit cell is 1, indicating that there must be an even number of spinons therein. Hence, the visons do not carry a fractional crystal momentum, and the vison translation commutes [42]. There will be two major differences of such fractional crystal momentum in the vison-pair continua at $m_z = 0$ and $\frac{1}{6}$.

First, consider the limit where the spectral edge in DSSF is dominated by scattering states of a pair of visons. If the vison carries a fractional crystal momentum, the density of the scattering states $N(q, \omega)$ should exhibit an enhanced periodicity $[19,20]$

$$N(q, \omega) = N(q + K, \omega),$$

where $K$ is half of the reciprocal vector, i.e., $2K = G$. In particular, such enhanced periodicity should manifest in the spectral edge.

Second, the translational symmetry fractionalization is also reflected on the gap-closing momenta near the phase transition driven by vison condensation. Phase transitions between the QSL and nearby symmetry-breaking phases can be understood as driven by anyon condensations: the transition to the FM phase is driven by spinon condensation, and that to the valence bond solid (VBS) phases, both transition to the FM phase is driven by spinon condensation, and the vison condensation. However, in (a), the enhanced periodicity manifests in that both points $\Gamma$ and $M$ become gapless due to the vison condensation. However, in (a), the enhanced periodicity manifests in that both points $\Gamma$ and $M$ become gapless, signifying translational symmetry fractionalization, whereas in (b), there is no enhanced periodicity and, hence, no translational symmetry fractionalization. Insets show the static structure factor of the two VBS phases for $m_z = 0$ and $\frac{1}{6}$, respectively, in (a), the Bragg peaks are at both $\Gamma$ and $M$, whereas in (b), only at $\Gamma$.

The sharp contrast in Fig. 3 between $m_z = 0$ and $\frac{1}{6}$, both in static and dynamic structure factors, clearly demonstrate the presence or absence of the translation symmetry fractionalization in $Z_2$ QSLs at the two magnetizations. This is, to our knowledge, for the first time, being observed in a nonperturbative manner. These results point out the possibility that inelastic neutron scattering or resonance (inelastic) x-ray scattering experiments can be further employed to identify gapped QSL on kagome magnets, e.g., in ZnCu$_3$(OH)$_6$Cl$_2$ (Herbertsmithite) [13,43] and Cu$_2$Zn(OH)$_6$FBr (Zn-doped Barlowite) [14,44–49]. In both cases, existing experimental data are pointing towards gapped QSL ground states with possibly $Z_2$ topological order, especially the latter, in which a gapped spinon continuum has been consistently revealed from both NMR [44] and inelastic neutron scattering experiments [14]. If, when driving the material through a transition from QSL to ordered state, the doubled period could be observed in DSSF, such a dynamical signature of symmetry fractionalization will be the decisive information to confirm the $Z_2$ QSL in materials.
Discussion.—Employing large-scale QMC + SAC simulations, we study the DSSF in extended BFG models at different magnetizations. We associate the DSSF of $S^zS^z$ and $S^+S^-$ operators with the two-particle continua of the vison and spinons. The two-vison continuum reveals the difference in translation-symmetry fractionalization between QSLs at different $m_z$: at $m_z = 0$, the continuum has an enhanced periodicity relating $\Gamma$ and $M$ points, meaning that the vison carries the symmetry fractionalization. In contrast, at $m_z = \frac{1}{2}$, the continuum has no such enhanced periodicity, meaning that the vison carries a trivial symmetry fractionalization, instead. Furthermore, at $m_z = 0$, this enhanced periodicity also implies that the condensation of visons must occur simultaneously at $\Gamma$ and $M$ and, thus, breaks translation symmetries. Correspondingly, the condensation of visons at $m_z = \frac{1}{2}$ leads to a translational symmetric VBS state [21]. Therefore, the dispersion of the two-vison continuum observed in the DSSF, together with the nature of the vison-condensation transition, reveals the symmetry fractionalization pattern of the anyonic excitations in QSL.

Our findings show that the DSSF can not only detect the existence of fractionalized anyonic excitations in a QSL, but also distinguish different symmetry-fractionalization patterns carried by the anyons. Since DSSF can be measured in different experimental probes, our findings not only have theoretical importance in understanding the properties of the topological state of matter, but also provide a valuable experimental guide to look for the dynamical signature of symmetry-enriched topological order in QSL materials.

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[34] H. Shao and A. W. Sandvik (to be published).
[42] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.121.077201 for details of the vison translational symmetry fractionalization, the consequential enhanced periodicity of density of states in DSSF, and the finite size effects in the obtained $S^{zz}(q, \omega)$ from the QMC + SAC simulations.