

Excitation spectrum of spin-1 Kitaev spin liquids

Yu-Hsueh Chen¹, Jozef Genzor¹, Yong Baek Kim², and Ying-Jer Kao^{1,3,*}

¹*Department of Physics and Center for Theoretical Physics, National Taiwan University, Taipei 10607, Taiwan*

²*Department of Physics, University of Toronto, Toronto, Ontario, Canada M5S 1A7*

³*Physics Division, National Center for Theoretical Science, National Taiwan University, Taipei 10607, Taiwan*



(Received 23 July 2021; revised 14 January 2022; accepted 24 January 2022; published 7 February 2022)

We study the excitation spectrum of the spin-1 Kitaev model using the symmetric tensor network. By evaluating the virtual order parameters defined on the virtual Hilbert space in the tensor network formalism, we confirm the ground state is in a $\mathbb{Z}_2$ spin-liquid phase. Using the correspondence between the transfer matrix spectrum and low-lying excitations, we find that contrary to the dispersive Majorana excitation in the spin-1/2 case, the isotropic spin-1 Kitaev model has a dispersive bosonic charge excitation. The bottom of the gapped single-particle charge excitations is found at $\mathbf{K}$, $\mathbf{K}' = (\pm 2\pi/3, \mp 2\pi/3)$, with a corresponding correlation length of $\xi \approx 6.7$ unit cells. The lower edge of the two-particle continuum, which is closely related to the dynamical structure factor measured in inelastic neutron scattering experiments, is obtained by extracting the excitations in the vacuum superselection sector in the anyon theory language.

DOI: [10.1103/PhysRevB.105.L060403](https://doi.org/10.1103/PhysRevB.105.L060403)

Quantum spin liquids (QSLs) are phases of matter characterized by the existence of long-range entanglement in the ground states and fractionalized excitations [1–3]. The exactly solvable model introduced by Kitaev [4] opens up a new avenue to search for QSL materials in nature that realize Kitaev-like interactions [5–11]. On the other hand, a higher-spin Kitaev model has also been theoretically studied, as the frustrated Ising-like interactions may provide an alternative route to access QSLs [12–14]. Recently, a microscopic mechanism to realize a $S = 1$ Kitaev model and candidate materials have been proposed [15], raising the importance of the study of higher-spin Kitaev physics. Different from its spin-1/2 counterpart, the higher-spin Kitaev model cannot be exactly solved by mapping the spins to Majorana fermions, and numerical studies have been carried out to identify the nature of the ground states for the $S = 1$ Kitaev model [16–21]. While several studies suggest that the isotropic spin-1 Kitaev model exhibits spin liquids with a $\mathbb{Z}_2$ gauge structure, quantitative features about the fractionalized excitations, i.e., the excitation spectrum, are still missing.

The excitation spectrum is deeply connected to the experiments. If the system harbors fractionalized excitations, the dynamical spin structure factor measured in inelastic neutron scattering (INS) should exhibit a broad continuum arising from multiparticle excitations [22]. In the two-dimensional (2D) system, gapped excitations of the QSLs are called anyons, and different types of anyons are distinguished by different superselection sectors [4,

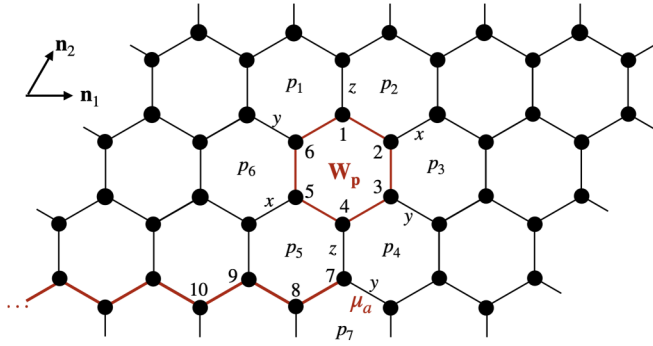


FIG. 1. Honeycomb lattice with the flux operator W_p defined on the plaquette p and the half-infinite string operator μ_a defined on the link $a = (7, y)$.

commutes with the Hamiltonian, where $U^\gamma = e^{i\pi S^\gamma}$. The Hilbert space is thus divided into sectors according to the eigenvalues of the flux operator $w_p = \pm 1$. In the isotropic case $J_x = J_y = J_z = 1$, the ground state lives in the vortex-free sector $w_p = +1, \forall p$ [12]. Therefore, the states with $w_p = -1$ for a given plaquette p can be understood as a $\mathbb{Z}_2$ vortex quasiparticle. On the other hand, one can define a half-infinite string operator $\mu_a = \prod_{n=1}^{\infty} (i)^{2S} U_n^\gamma$ labeled by $a = (i, \gamma)$ for a given link γ attached to site i . Here, $(i, i+1, \dots)$ are sites traversed by the string and $(\gamma_i, \gamma_{i+1}, \dots)$ are links normal to the string. For instance, the string operator μ_a with $a = (7, y)$ in Fig. 1 is $\prod_{n=7}^{\infty} (i)^{2S} U_n^y$. In the vortex-free sector, the path of the string is irrelevant since one can deform the path by applying W_p without changing the wave function. Therefore, one can regard the starting point of the string operator as a topologically nontrivial excitation. This operator is the same disorder operator defined in Ref. [12], where by attaching specific operators to the starting point of μ_a , one can construct a set of operators acting as Majorana fermions and hard-core bosons for the half-integer and integer spin, respectively.

The qualitative difference between the integer and half-integer Kitaev models can be understood through the identities

$$U^\alpha U^\beta = \begin{cases} \delta^{\alpha\beta} \mathbb{I} + |\epsilon^{\alpha\beta\gamma}| U^\gamma, & S = 0, 1, \dots, \\ -\delta^{\alpha\beta} \mathbb{I} + \epsilon^{\alpha\beta\gamma} U^\gamma, & S = 1/2, 3/2, \dots, \end{cases} \quad (2)$$

where $\epsilon^{\alpha\beta\gamma}$ is the Levi-Civita symbol. Consider moving a $\mathbb{Z}_2$ vortex around the central plaquette p with $w_p = -1$ following the path $p_1 \rightarrow p_2 \rightarrow \dots \rightarrow p_6$ in Fig. 1. For the half-integer spin, the action of moving the vortex from p_1 to p_2 can be done by U_1^z since $\{W_{p_1}, U_1^z\} = \{W_{p_2}, U_1^z\} = 0$ due to the relation $\{U_1^y, U_1^z\} = \{U_1^x, U_1^z\} = 0$. Therefore, the operator moving a $\mathbb{Z}_2$

the ITE, we apply the LG projector at the end to obtain a $\mathbb{Z}_2$ -invariant ground state. In other words, we first perform the ITE and then apply the LG projector to the resulting state, i.e., $|\psi\rangle = \lim_{\tau \rightarrow \infty} Q_{LG} e^{-\tau H} |\psi_0\rangle$. Here, the initial product state $|\psi_0\rangle = \otimes_\alpha |(111)\rangle_\alpha$, where $|(111)\rangle$ is the magnetized state along the (1,1,1) direction. This ensures that the PEPS with a fixed bond dimension D is vortex free and satisfies all the nice properties inherited from the LG projector. Another interesting property of this construction is that $S^z Q_{kij} = \sum_{k'} \sigma_{kk'}^z Q_{k'ij} S^z$ (and similar relations for S^x, S^y) [Fig. 2(e)], which indicates that S^z will not only move the vortex but change the ITE wave function to $S^z e^{-\tau H} |\psi_0\rangle$, making the previous argument that the loop operator $S_1^z S_2^x S_3^y S_4^z S_5^y S_6^y$ will change the ground state more obvious. It is the LG projector that allows us to manipulate the vortex on the virtual bonds using σ^z without spoiling the wave function. In addition, our construction allows for a lower computational cost than that of the gauge-symmetry-preserved update [31,32], as only half of the bond dimension is needed during the ITE process.

While the LG projector forms a natural framework to describe $\mathbb{Z}_2$ QSLs, the topological property of the projected wave function also depends on the initial trial state. For instance, it is possible to have $|\psi\rangle = \mu_a |\psi\rangle$ for some state $|\psi\rangle = Q_{LG} |\psi_{\text{trial}}\rangle$. In this case, the half-infinite string operator μ_a which should create a charge anyon actually does nothing to the ground state, and thus the charge is condensed. Similarly, if $\langle \psi_{\text{ex}} | \psi_{\text{ex}} \rangle = 0$, the system is in a charge confined phase [28,29,33]. Therefore, to nail down the nature of the isotropic spin-1 Kitaev model, one should make sure μ_a actually creates a proper excitation. In other words, we should consider the overlap of the wave functions $\langle \psi_{\text{ex}} | \psi_{\text{ex}} \rangle$ and $\langle \psi_{\text{ex}} | \psi \rangle$ where $|\psi_{\text{ex}}\rangle = \mu_a |\psi\rangle$.

As stated previously, the effect of μ_a is equivalent to applying a local σ^x on the virtual bond using the physical-virtual relation in Fig. 2(c); therefore, the overlap of the charge excited state can be evaluated easily in the virtual Hilbert space. To calculate those quantities, we consider the transfer matrix (TM) $\mathbb{T} \equiv \lim_{L_x \rightarrow \infty} \text{tTr}(\mathbb{E}^1 \mathbb{E}^2 \cdots \mathbb{E}^{L_x})$ with $\mathbb{E}$ the double tensor formed by contracting the physical indices of the local tensor A and its adjoint A^* . The TM can be regarded as the building block of the norm of the two-dimensional PEPS, $\langle \psi | \psi \rangle = (l | \lim_{L_y \rightarrow \infty} \mathbb{T}^{L_y} | r) = (l | [\lim_{L_y \rightarrow \infty} |l\rangle \lambda^{L_y} (r)] | r)$, where $|l\rangle$ ($|r\rangle$) is the left (right) dominant eigenvector of $\mathbb{T}$ and λ is the corresponding dominant eigenvalue which is normalized to 1. Here, we use $|\cdot\rangle$ to denote a vector defined in the virtual Hilbert space. In our case, $|l\rangle$ and $|r\rangle$ are the same and we denote them as $|\rho\rangle$ in the following. It is then obvious that the overlap of the wave functions $\langle \psi_{\text{ex}} | \psi \rangle$ and $\langle \psi_{\text{ex$

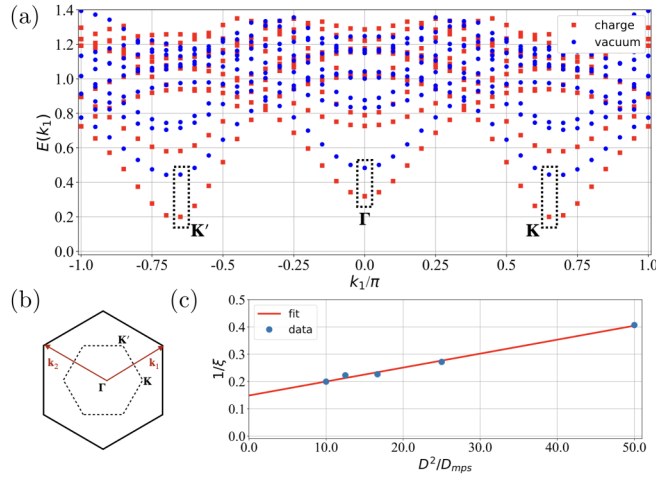


FIG. 3. (a) Transfer matrix spectrum for the PEPS tensor with $(D, D_{\text{mps}}) = (10, 10)$. (b) Brillouin zone with labeled positions of the minimum of TM spectrum. (c) The inverse of the correlation length of the $D = 10$ PEPS wave function as a function of D_{mps} .

by distinguishing the TM spectrum with appropriate quantum numbers defined on the virtual Hilbert space [30].

Interestingly, for the spin-1 Kitaev model, we find that $\lambda_{(I|m)} = \lambda_{(I|\epsilon)} = 0$, indicating there are no TM excitations belonging to the $\mathbb{T}_{(I|m)}$ and $\mathbb{T}_{(I|\epsilon)}$ sectors. This shows that the LG projector for the integer spins only supports dispersive excitations belonging to the vacuum and charge sectors, while the flux- and fermion-sector excitations are static. This is intrinsically different from the half-integer LG projector, where only vacuum and fermion excitations are dispersive [44]. In addition, this is consistent with the argument put forth in Ref. [12] that the integer-spin Kitaev model has bosonic excitations instead of Majorana fermions, indicating that the different sign structures of the integer and half-integer spin LG projectors may faithfully describe the distinct nature of the integer and half-integer spin Kitaev models [21].

Using the correspondence $E_{k_1} \sim -\log |\lambda_{k_1}|$ for a given momentum k_1 in the x direction, the TM spectra for PEPS states with bond dimension $D = 10$ are shown in Fig. 3(a). The excitations belonging to charge and vacuum sectors are labeled by red and blue colors, respectively. While the overall energy scale of the minimum of E_{k_1} and exact excitation energies are unknown due to the lack of the knowledge of the Lieb-Robinson velocity [45], the corresponding momentum k_1 at the local minimum of E_{k_1} allows us to identify the location of the low-energy dispersion [41]. It then follows that both the charge- and vacuum-sector excitations are clearly identified at $k_1 = 0, 2\pi/3$, and $-2\pi/3$. We also perform the corner transfer matrix renormalization group (CTMRG) [46–48] to obtain the TM spectrum [30], and the results are consistent. To gain more insights into the two-dimensional system, we consider the momentum in the y direction using $k_2 \sim \arg \lambda_{k_1}$. The locations of three minimum excitations are then identified at

$(k_1, k_2) = (0, 0)$, $(2\pi/3, -2\pi/3)$, and $(-2\pi/3, 2\pi/3)$, suggesting that the spin-1 Kitaev model harbors three low-lying charge anyon excitations at the Γ , $\mathbf{K}$, and $\mathbf{K}'$ points in the Brillouin zone [Fig. 3(b)]. To nail down the origin of the vacuum-sector excitations, which correspond to all possible even-particle excitations, we note that the global minima lie at $\mathbf{K}$ ($\mathbf{K}'$):

- [3] C. Broholm, R. J. Cava, S. A. Kivelson, D. G. Nocera, M. R. Norman, and T. Senthil, Quantum spin liquids, *Science* **367**, 6475 (2020).
- [4] A. Kitaev, Anyons in an exactly solved model and beyond, *Ann. Phys.* **321**, 2 (2006).
- [5] G. Jackeli and G. Khaliullin, Mott Insulators in the Strong Spin-Orbit Coupling Limit: From Heisenberg to a Quantum Compass and Kitaev Models, *Phys. Rev. Lett.* **102**, 017205 (2009).
- [6] Y. Singh, S. Manni, J. Reuther, T. Berlijn, R. Thomale, W. Ku, S. Trebst, and P. Gegenwart, Relevance of the Heisenberg-Kitaev Model for the Honeycomb Lattice Iridates $A_2\text{IrO}_3$, *Phys. Rev. Lett.* **108**, 127203 (2012).
- [7] W. Witczak-Krempa, G. Chen, Y. B. Kim, and L. Balents, Correlated quantum phenomena in the strong spin-orbit regime, *Annu. Rev. Condens. Matter Phys.* **5**, 57 (2014).
- [8] J. G. Rau, E. K.-H. Lee, and H.-Y. Kee, Spin-orbit physics giving rise to novel phases in correlated systems: Iridates and related materials, *Annu. Rev. Condens. Matter Phys.* **7**, 195 (2016).
- [9] S. M. Winter, A. A. Tsirlin, M. Daghofer, J. van den Brink, Y. Singh, P. Gegenwart, and R. Valentí, Models and materials for generalized Kitaev magnetism, *J. Phys.: Condens. Matter* **29**, 493002 (2017).
- [10] K. W. Plumb, J. P. Clancy, L. J. Sandilands, V. V. Shankar, Y. F. Hu, K. S. Burch, H.-Y. Kee, and Y.-J. Kim, $\alpha\text{-RuCl}_3$: A spin-orbit assisted Mott insulator on a honeycomb lattice, *Phys. Rev. B* **90**, 041112(R) (2014).
- [11] Y. Kasahara, T. Ohnishi, Y. Mizukami, O. Tanaka, S. Ma, K. Sugii, N. Kurita, H. Tanaka, J. Nasu, Y. Motome *et al.*, Majorana quantization and half-integer thermal quantum Hall effect in a Kitaev spin liquid, *Nature (London)* **559**, 227 (2018).
- [12] G. Baskaran, D. Sen, and R. Shankar, Spin- S Kitaev model: Classical ground states, order from disorder, and exact correlation functions, *Phys. Rev. B* **78**, 115116 (2008).
- [13] T. Minakawa, J. Nasu, and A. Koga, Quantum and classical behavior of spin- S Kitaev models in the anisotropic limit, *Phys. Rev. B* **99**, 104408 (2019).
- [14] J. Oitmaa, A. Koga, and R. R. P. Singh, Incipient and well-developed entropy plateaus in spin- S Kitaev models, *Phys. Rev. B* **98**, 214404 (2018).
- [15] P. P. Stavropoulos, D. Pereira, and H.-Y. Kee, Microscopic Mechanism for a Higher-Spin Kitaev Model, *Phys. Rev. Lett.* **123**, 037203 (2019).
- [16] A. Koga, H. Tomishige, and J. Nasu, Ground-state and

- [40] S. Hu, W. Zhu, S. Eggert, and Y.-C. He, Dirac Spin Liquid on the Spin-1/2 Triangular Heisenberg Antiferromagnet, *Phys. Rev. Lett.* **123**, 207203 (2019).
- [41] M. B. Hastings, Locality in Quantum and Markov Dynamics on Lattices and Networks, *Phys. Rev. Lett.* **93**, 140402 (2004).
- [42] J. Haegeman, B. Pirvu, D. J. Weir, J. I. Cirac, T. J. Osborne, H. Verschelde, and F. Verstraete, Variational matrix product ansatz for dispersion relations, *Phys. Rev. B* **85**, 100408(R) (2012).
- [43] Y. Zhang, T. Grover, A. Turner, M. Oshikawa, and A. Vishwanath, Quasiparticle statistics and braiding from ground-state entanglement, *Phys. Rev. B* **85**, 235151 (2012).
- [44] Y.-H. Chen, C.-Y. Huang, and Y.-J. Kao, Detecting transition between Abelian and non-Abelian topological orders through symmetric tensor networks, *Phys. Rev. B* **104**, 045131 (2021).
- [45] E. H. Lieb and D. W. Robinson, The finite group velocity of quantum spin systems, *Commun. Math. Phys.* **28**, 251 (1972).
- [46] T. Nishino and K. Okunishi, Corner transfer matrix renormalization group method, *J. Phys. Soc. Jpn.* **65**, 891 (1996).
- [47] R. Orús and G. Vidal, Simulation of two-dimensional quantum systems on an infinite lattice revisited: Corner transfer matrix for tensor contraction, *Phys. Rev. B* **80**, 094403 (2009).
- [48] P. Corboz, J. Jordan, and G. Vidal, Simulation of fermionic lattice models in two dimensions with projected entangled-pair states: Next-nearest neighbor Hamiltonians, *Phys. Rev. B* **82**, 245119 (2010).
- [49] G. Baskaran, S. Mandal, and R. Shankar, Exact Results for Spin Dynamics and Fractionalization in the Kitaev Model, *Phys. Rev. Lett.* **98**, 247201 (2007).
- [50] J. Knolle, D. L. Kovrizhin, J. T. Chalker, and R. Moessner, Dynamics of a Two-Dimensional Quantum Spin Liquid: Signatures of Emergent Majorana Fermions and Fluxes, *Phys. Rev. Lett.* **112**, 207203 (2014).
- [51] J. Knolle, D. L. Kovrizhin, J. T. Chalker, and R. Moessner, Dynamics of fractionalization in quantum spin liquids, *Phys. Rev. B* **92**, 115127 (2015).
- [52] G. B. Halász, N. B. Perkins, and J. van den Brink, Resonant Inelastic X-ray Scattering Response of the Kitaev Honeycomb Model, *Phys. Rev. Lett.* **117**, 127203 (2016).
- [53] M. Gohlke, R. Verresen, R. Moessner, and F. Pollmann, Dynamics of the Kitaev-Heisenberg Model, *Phys. Rev. Lett.* **119**, 157203 (2017).