Analytic calculation of the vison gap in the Kitaev spin liquid

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Although the ground-state energy of the Kitaev spin liquid can be calculated exactly, the associated vison gap energy has to date only been calculated numerically from finite size diagonalization. Here we show that the phase shift for scattering Majorana fermions off a single bond flip can be calculated analytically, leading to a closed-form expression for the vison gap energy $\Delta = 0.2633J$. Generalizations of our approach can be applied to Kitaev spin liquids on more complex lattices such as the three-dimensional hyperoctagonal lattice.

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I. INTRODUCTION

Kitaev spin liquids (KSL) are a class of exactly solvable quantum spin liquids that exhibit spin fractionalization, anyonic excitations, and long-range entanglement [1–5]. The fractionalization of spins into Majorana fermions is accompanied by the formation of emergent $\mathbb{Z}_2$ gauge fields, giving rise to $\mathbb{Z}_2$ vortex excitations or "visons." These excitations are gapped and the energy cost associated with creating two visons on adjacent plaquettes is called the vison gap Δ_v (Fig. 1). Proposals for the practical realization of Kitaev spin liquids in quantum materials, including α-$RuCl_3$ [5–14] and iridates [11,15,16], have renewed interest in the thermodynamics of Kitaev spin liquid [17–24]. The extension of these ideas to Yao-Lee spin liquid [25,26] and its application to Kondo models [27,28] motivate the development of an analytical approach to calculate the vison gap Δ_v.

The vison gap in KSLs has to date been determined by numerical diagonalization of finite size systems [1,3]. Here we present a Green's function approach for the analytical computation of the vison gap Δ_v from the scattering phase shift associated with a $\mathbb{Z}_2$ bond flip. Our work builds on theoretical developments in the field of Kitaev spin liquids which relate to the interplay between Majorana fermions and visons [1,19,29–37]. Using exact calculations, we find the vison gap energy of $\Delta_v = 0.263313(6)J$ for the Kitaev spin liquid on honeycomb lattice in the gapless phase, extending the accuracy of previous calculations [1,3]. Our calculations reveal the formation of Majorana resonances in the density of states which accompany the formation of two adjacent visons. Our approach can be simply generalized to more complex lattices and are immediately generalizable to Yao-Lee spin liquids.

II. VISON GAP IN THE KITAEV HONEYCOMB MODEL

The Kitaev honeycomb lattice model [1] is described by the Hamiltonian

$$H_K = \sum_{\langle ij\rangle} J_{\alpha_{ij}} \sigma_i^{\alpha_{ij}} \sigma_j^{\alpha_{ij}}, \tag{1}$$

where the Heisenberg spins $\vec{\sigma}_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$ at site i interact with their nearest neighbors via an Ising coupling between the $\alpha_{ij} = x, y, z$ spin components, along the corresponding bond directions $\langle ij\rangle$, with strength $J_{\alpha_{ij}}$, as shown in Fig. 1. An exact solution of the Kitaev model [1] is found by representing the spins as products of Majorana fermions, $\sigma_j^\alpha = 2ic_j b_j^\alpha$, which satisfy canonical anticommutation algebras, $\{c_i, b_j^\alpha\} = 0$, $\{b_i^\alpha, b_j^\beta\} = \delta_{ij}\delta^{\alpha,\beta}$ [taking the convention that $c_j^2 = (b_j^\alpha)^2 = 1/2$]. The system is projected into the physical subspace by selecting $\mathcal{D}_j \equiv -4ic_j b_j^x b_j^y b_j^z = 1$ at each site, allowing the Hamiltonian (1) to be rewritten as $\mathbb{Z}_2$ gauge theory

$$H_{\rm KSL} = 2\sum_{\langle ij\rangle} J_{\alpha_{ij}} \hat{u}_{ij} (ic_i c_j), \tag{2}$$

where the gauge fields $\hat{u}_{ij} = 2ib_i^{\alpha_{ij}} b_j^{\alpha_{ij}} = \pm 1$ on bond ij commute with the Hamiltonian, $[\hat{u}_{ij}, H_K] = 0$. The plaquette operators $\mathcal{W}_p$

$$\mathcal{W}_p = \prod_{\langle i,j\rangle \in p} u_{ij} \quad (i \in A,\, j \in B), \tag{3}$$

formed from the product of gauge fields $\hat{u}_{ij}$ around the hexagonal loop p (plaquette), are gauge invariant and also commute with the Hamiltonian $[\mathcal{W}_p, H_K] = 0$ and constraint operators $[\mathcal{W}_p, \mathcal{D}_j] = 0$, giving rise to a set of static constants of motion which take values $\mathcal{W}_p = \pm 1$. Each eigenstate is characterized by the configurations of $\{\mathcal{W}_p\}$; Lieb's theorem [38] specifies that the ground state configuration is flux free, i.e., $\mathcal{W}_p = 1$ for all hexagons p. In what follows we will choose the gauge $\hat{u}_{ij} = 1$ when $i \in A$ and $j \in B$ sublattice, assigning

$$H_0 = H_{\rm KSL}[u_{ij} \to 1]. \tag{4}$$

Rewriting H_0 in momentum space, we obtain

$$H_0 = \frac{1}{2}\sum_{\mathbf{k}\in \mathbf{BZ}} \psi_{\mathbf{k}}^\dagger (\vec{\gamma}_{\mathbf{k}} \cdot \vec{\tau}) \psi_{\mathbf{k}}, \tag{5}$$

where

$$\psi_{\mathbf{k}} = \frac{1}{\sqrt{N_c}} \sum_j \begin{pmatrix} c_{j,A} \\ c_{j,B} \end{pmatrix} e^{-i\mathbf{k}\cdot\mathbf{R}_j} \tag{6}$$

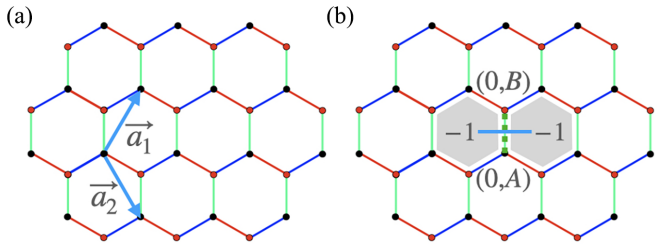

FIG. 1. (a) Kitaev honeycomb lattice model, where the Ising spin couplings along the x, y, and z directions are labeled by blue, green, and red bonds, respectively, with primitive lattice vectors $\vec{a}_1$ and $\vec{a}_2$. (b) A bond reversal at the origin creates a vison pair, costing an energy Δ_v. The string connecting the adjacent visons is indicated in light blue.

describes a Majorana in momentum space, where N_c is the number of unit cells and $\mathbf{R}_j$ is the location of the unit cell and $\vec{\gamma}_\mathbf{k} = [\mathrm{Re}(\gamma_\mathbf{k}), -\mathrm{Im}(\gamma_\mathbf{k})]$ is expressed in terms of the form factor

$$\gamma_\mathbf{k} = 2i\left(J_z + J_x e^{ik_1} + J_y e^{ik_2}\right),$$
$$\mathbf{k} = \frac{k_1}{2\pi}\mathbf{b_1} + \frac{k_2}{2\pi}\mathbf{b_2}, \quad k_1, k_2 \in [0, 2\pi]. \tag{7}$$

Here we have employed a reciprocal lattice basis $\mathbf{b_1}, \mathbf{b_2}$ to span the momentum $\mathbf{k} \in \mathbf{BZ}$, which transforms to a rhombus shaped Brillouin zone in the reciprocal lattice (see Fig. 2). The Majorana excitation spectrum of the Kitaev spin liquid is given by the eigenvalues of H_0, $\epsilon_\mathbf{k} = \pm|\gamma_\mathbf{k}|$.

We create two adjacent visons by flipping the gauge field in the unit cell at origin to $\hat{u}_{(0,A)(0,B)} = -1$ as shown in Fig. 1, resulting in the following Hamiltonian:

$$H_{\mathrm{KSL}+2v} = H_0 + \hat{V}, \tag{8}$$

where

$$\hat{V} = -4J_z(ic_{0,A}c_{0,B}) \tag{9}$$

acts as a scattering term for Majoranas in the bulk. In this way, the vison gap calculation is formulated as a scattering problem.

For this case, the Hamiltonian is given by

$$H_{\mathrm{KSL}+2v} = \frac{1}{2}\sum_{\mathbf{k}\in\mathbf{BZ}} \psi^\dagger_\mathbf{k}(\vec{\gamma}_\mathbf{k}\cdot\vec{\tau})\psi_\mathbf{k} + \frac{1}{2}\mathbf{c}_0^T(V\tau_2)\mathbf{c}_0, \tag{10}$$

$$\mathbf{c}_0 = \begin{pmatrix} c_{0,A} \\ c_{0,B} \end{pmatrix} = \frac{1}{\sqrt{N_c}}\sum_{\mathbf{k}\in\mathbf{BZ}} \psi_\mathbf{k}, \tag{11}$$

describes a Majorana fermion at the origin, and $V = 4J_z$.

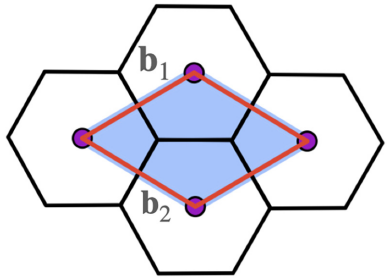

FIG. 2. Rearranged first Brillouin zone (BZ) constructed in the reciprocal lattice vector basis spanned by $\mathbf{b_1}$ and $\mathbf{b_2}$.

We now set up the scattering problem in terms of Green's functions. The Green's function of the unscattered Majoranas is $G_0 = G_0(i\omega_n, \mathbf{k})\delta_{\mathbf{k},\mathbf{k}'}$, where

$$G_0(i\omega_n, \mathbf{k}) = [i\omega_n - \vec{\gamma}_\mathbf{k}\cdot\vec{\tau}]^{-1}. \tag{12}$$

In the presence of the bond flip at the origin, the Green's function of the scattered Majoranas is given by $G = (G_0^{-1} - \hat{V})^{-1}$, where $\hat{V}_{\mathbf{k},\mathbf{k}'} = (V\tau_2)/N_c$ is the scattering matrix. The total free energy of the noninteracting ground state in the presence of the scattering is given by the standard formula

$$\beta F = -\tfrac{1}{2}\mathrm{Tr}[\ln(-G^{-1})] = -\tfrac{1}{2}\mathrm{Tr}\,\ln[-G_0^{-1} + \hat{V}], \tag{13}$$

where Tr denotes the full trace over Matsubara frequencies, momenta, and sublattice degrees of freedom. The change in free energy is then given by

$$\beta\Delta F = -\frac{1}{2}\mathrm{Tr}[\ln(1 - \hat{V}G_0)] = \frac{1}{2}\sum_{r=1}^{\infty}\frac{1}{r}\mathrm{Tr}[(\hat{V}G_0)^r]. \tag{14}$$

We now carry out the trace over the Matsubara frequencies and momenta, so that

$$\Delta F = \frac{1}{2\beta}\sum_{i\omega_n}\sum_{r=1}^{\infty}\frac{1}{r}\mathrm{tr}\left[\left(\frac{V\tau_2}{N_c}\sum_{\mathbf{k}} G_0(i\omega_n, \mathbf{k})\right)^r\right], \tag{15}$$

where tr[ ] denotes the residual trace over sublattice degrees of freedom. Now, we can incorporate the summations over momentum by introducing the local Green's function

$$g(z) = \frac{1}{N_c}\sum_{\mathbf{k}\in\mathbf{BZ}} G_0(z, \mathbf{k}), \tag{16}$$

so that

$$\Delta F = \frac{1}{2\beta}\sum_{i\omega_n}\sum_{r=1}^{\infty}\frac{1}{r}\mathrm{tr}\{[V\tau_2 g(i\omega_n)]^r\}$$
$$= -\frac{1}{2\beta}\sum_{i\omega_n}\mathrm{tr}\{\ln[1 - V\tau_2 g(i\omega_n)]\}, \tag{17}$$

where we have reassembled the Taylor series as a logarithm.

We shall illustrate our method for the isotropic case $J_x = J_y = J_z = J$, setting $K = 2J$ and $V = 4J$. In this case, $\gamma_\mathbf{k} = iK(1 + e^{ik_1} + e^{ik_2})$. If we divide $\gamma_\mathbf{k} = i[\gamma_c(\mathbf{k}) + i\gamma_s(\mathbf{k})]$ into its even and odd components

$$\gamma_c(\mathbf{k}) = K(1 + \cos k_1 + \cos k_2),$$
$$\gamma_s(\mathbf{k}) = K(\sin k_1 + \sin k_2), \tag{18}$$

then $g(i\omega_n)$ can be rewritten as

$$g(z) = \frac{1}{N_c}\sum_{\mathbf{k}\in\mathbf{BZ}}\frac{z - [\gamma_c(\mathbf{k})\tau_2 + \gamma_s(\mathbf{k})\tau_1]}{z^2 - |\gamma_\mathbf{k}|^2}. \tag{19}$$

The odd component $\gamma_s(\mathbf{k})$ vanishes under momentum summation so that

$$1 - \hat{V}g(z) = 1 - \frac{V}{N_c}\sum_{\mathbf{k}\in\mathbf{BZ}}\frac{z\tau_2 - \gamma_c(\mathbf{k})}{z^2 - |\gamma_\mathbf{k}|^2}$$
$$= 1 - V[\tau_2 g_0(z) - \mathbb{I}_2 g_2(z)], \tag{20}$$

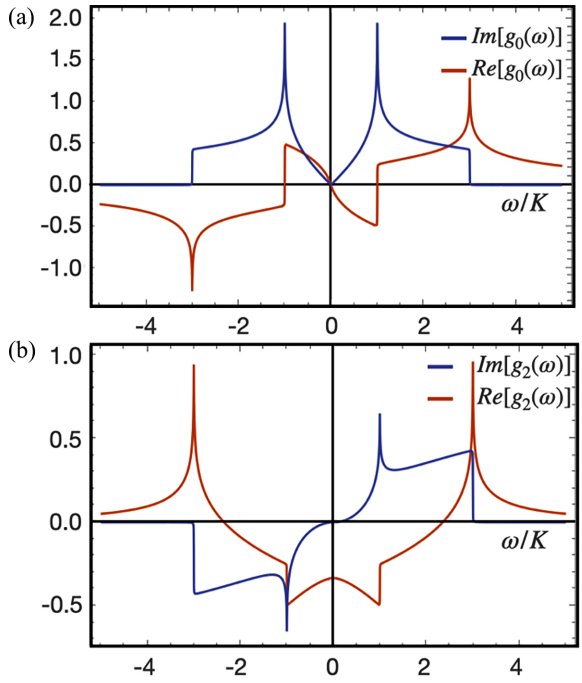

FIG. 3. Showing real and imaginary parts of (a) $g_0(\omega - i\delta)$ and (b) $g_2(\omega - i\delta)$ as defined in Eqs. (21), (27), and (28).

where

$$g_0(z) \equiv \frac{1}{N_c}\sum_{\mathbf{k}\in\mathbf{BZ}} \frac{z}{z^2 - |\gamma_\mathbf{k}|^2},$$
$$g_2(z) \equiv \frac{1}{N_c}\sum_{\mathbf{k}\in\mathbf{BZ}} \frac{\gamma_c(\mathbf{k})}{z^2 - |\gamma_\mathbf{k}|^2}. \tag{21}$$

Carrying out the trace in the free energy we then obtain

$$\Delta F = -\frac{T}{2}\mathrm{Tr}[\ln(1 - \hat{V}G_0)]$$
$$= -\frac{T}{2}\sum_{i\omega_n} \ln\{[1 + Vg_2(i\omega_n)]^2 - [Vg_0(i\omega_n)]^2\}. \tag{22}$$

The Matsubara summation can then be carried out as an counterclockwise contour integral around the imaginary axis weighted by Fermi function, $f(z) = [e^{\beta z} + 1]^{-1}$. Deforming the contour to run clockwise around the real axis we obtain

$$\Delta F = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\left(\frac{1}{2} - f(\omega)\right)\delta_v(\omega), \tag{23}$$

where

$$\delta_v(\omega) = \mathrm{Im}\ \ln\left[[1 + 2Kg_2(z)]^2 - [2Kg_0(z)]^2\right]_{z=\omega-i\delta} \tag{24}$$

is identified as the scattering phase shift, and $g_0(z)|_{z-\omega-i\delta}$ and $g_2(z)|_{z-\omega-i\delta}$ are the components of the local Green's function $g(z)|_{z=\omega-i\delta}$ (see Fig. 3). Note that $\delta_v(\omega) = -\delta_v(-\omega)$ is an antisymmetric function of frequency. At zero temperature the vison gap is then

$$\Delta_v = K\int_0^{\infty} \frac{dx}{2\pi}\ \mathrm{Im}\ \ln\left[[1 + 2g_2(z)]^2 - [2g_0(z)]^2\right]_{z=x-i\delta}, \tag{25}$$

where we have rescaled the frequency in units of K, setting $z = \omega/K$. In the reciprocal basis

$$g_0(z) = \int_0^{2\pi}\frac{dk_1}{2\pi}\int_0^{2\pi}\frac{dk_2}{2\pi}\frac{z}{z^2 - |\gamma_\mathbf{k}|^2},$$
$$g_2(z) = \int_0^{2\pi}\frac{dk_1}{2\pi}\int_0^{2\pi}\frac{dk_2}{2\pi}\frac{\gamma_c(\mathbf{k})}{z^2 - |\gamma_\mathbf{k}|^2}, \tag{26}$$

where we have set $K = 1$ in $\gamma(\mathbf{k})$, i.e., $\gamma_\mathbf{k} = 1 + e^{ik_1} + e^{ik_2}$ and $\gamma_c = \cos(k_1) + \cos(k_2)$. The interior integral over k_2 can be carried out as a complex contour integral over $w = e^{ik_2}$ around the unit circle (Appendix A), giving

$$g_0(z) = \int_0^{2\pi}\frac{dk}{2\pi}\frac{z}{[z^2 - (3 + 2c)]\sqrt{1 - \frac{8(c+1)}{[z^2-(3+2c)]^2}}}, \tag{27}$$

$$g_2(z) = \int_0^{2\pi}\frac{dk}{2\pi}\frac{2c + 1}{[z^2 - (3 + 2c)]\sqrt{1 - \frac{8(c+1)}{[z^2-(3+2c)]^2}}}, \tag{28}$$

where $c \equiv \cos(k)$. These integrals were evaluated numerically to obtain the phase shift $\delta_v(\omega)$ (Fig. 4). The phase shift was interpolated over a discrete set of N points and the integral (25) was carried out numerically on the interpolated phase shift. By extrapolating the limit $1/N \to 0$, we find the vison gap energy to be $\Delta_v = 0.1311656(3)$ K $= 0.263313(6)$ J for the isotropic case $J_z = J_y = J_z = J$.

This analytically based calculation improves on the earlier result obtained via numerical diagonalization of finite size systems [1], i.e., $\Delta_v \approx 0.267$ J. Its main virtue however, is that the method can be easily generalized, and we gain insights from the calculated scattering phase shifts.

From the calculated phase shift, we can calculate the change in density of states (DOS) (see Appendix B)

$$\Delta\rho(\omega) = \frac{1}{\pi}\frac{d\delta_v}{d\omega} \tag{29}$$

[Fig. 4(c)] associated with a bond flip, which is seen to contain a resonance centered around $\epsilon_0 \approx \pm 0.07$ K. This resonance can be examined in detail by expanding $g_0(z)$ and $g_2(z)$ for small z:

$$g_0(\omega - i\delta) = \frac{\omega}{\sqrt{3}\pi}\ln\left(\frac{3}{|\omega|}\right) + i\frac{|\omega|}{\sqrt{3}},$$
$$g_2(\omega - i\delta) = -\frac{2}{3} - \frac{\omega^2}{3\sqrt{3}\pi}\left[\ln\left(\frac{3}{|\omega|}\right) + i\pi\ \mathrm{sgn}\ \omega\right], \tag{30}$$

which can be used to evaluate scattering phase shift $\delta_v(\omega)$ (24) and the resonant DOS change $\Delta\rho(\omega)$ (29) analytically. The position of the resonance is determined by the integration over the entire band but its width is determined by the density of states at low energies. Since the DOS vanishes inside the spectral gap, the resonance will become sharp in the gapped topological phase when its center lies beneath the gap edge (see Fig. 5). The sharp peak in the gapped state signifies the binding of Majorana fermions to the visons formed by the $\mathbb{Z}_2$ bond flip at origin.

III. DISCUSSION

In this work we have presented an analytical method for determination of the vison gap by treating the flipping of

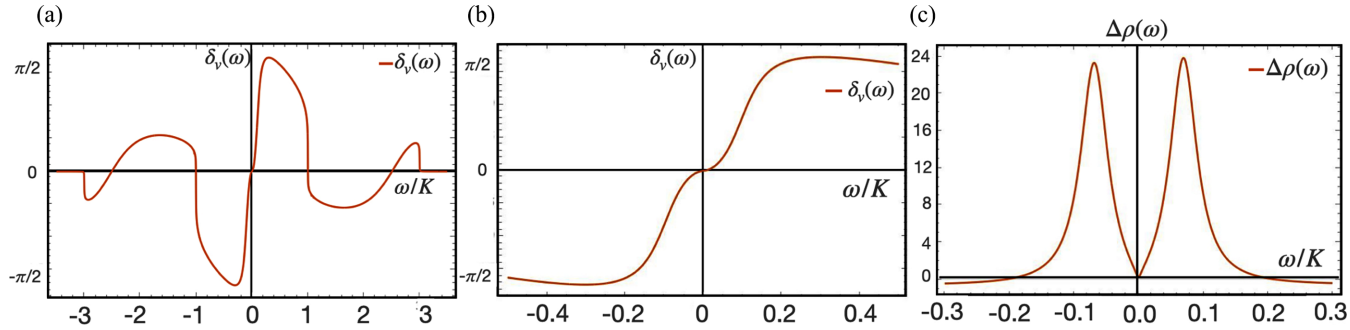

FIG. 4. (a) Scattering phase shift $\delta_v(\omega)$ associated with the creation of two adjacent visons, as a function of frequency ω in units of K. (b) Scattering phase shift $\delta_v(\omega)$ on an expanded scale, showing inflection point at origin. (c) Resonance in the scattering density of states around $\epsilon_0 = \pm 0.07$ K in the density of state change $\Delta\rho(\omega)$ due to the bond flip potential, as a function of frequency ω in units of K. This resonance will become sharp in the gapped topological state, when the resonance drops below the gap edge, forming a sharp, in-gap excitation of the vison pair.

the $\mathbb{Z}_2$ gauge field as a scattering potential for the Majorana fermions. In this way, we have been able to analytically extend the numerical treatment by Kitaev for the isotropic model on honeycomb lattice [1] to obtain an analytic result for the vison gap energy Δ_v.

A key part of our approach is the calculation of the Majorana phase shift for scattering off the bond-flipped configuration. One of the interesting observations is that the scattering contains a Majorana resonance, located at an energy $\epsilon_0 \approx \pm 0.07$ K. Since this resonance is formed from scattering throughout the entire Brillouin zone, its location is robust. Thus in those cases where the excitation spectrum acquires a gap, e.g., through time-reversal symmetry breaking [1,39], this resonance transforms into a sharp in-gap excitation.

While it is possible to extend our method to analytically calculate the energy associated with the injection of an anyon into the torus, by flipping $x-x$ bonds along $\mathbf{a_1}$ direction (see Fig. 6), a much simpler derivation of the anyon energy in the KSL can be made by taking two copies of the KSL,

$$H_{\mathrm{KSL},1} = 2\sum_{\langle ij\rangle} J_{\alpha_{ij}}\hat{u}_{ij}(ic_{1i}c_{1j}),$$
$$H_{\mathrm{KSL},2} = 2\sum_{\langle ij\rangle} J_{\alpha_{ij}}\hat{u}_{ij}(ic_{2i}c_{2j}), \tag{31}$$

forming a complex fermion Hamiltonian $H_c = H_{\mathrm{KSL},1} + H_{\mathrm{KSL},2} = 2\sum_{\langle ij\rangle} J_{\alpha_{ij}}\hat{u}_{ij}(ic_i^\dagger c_j + \mathrm{H.c})$, where $c_i \equiv (c_{1i} + ic_{2i})/\sqrt{2}$ is a complex fermion. The ground state excitation energy of H_c corresponding to the gauge configuration where one reverses $x-x$ bonds along the $\mathbf{a_1}$ direction is twice the anyon energy for H_{KSL}. For H_c the line of reverse bonds around the torus can then be absorbed by a unitary transformation that redistributes the odd boundary condition into an effective vector potential that shifts all the momenta $\mathbf{k} = (k_1, k_2) \to (k_1 + \frac{\pi}{L}, k_2)$ equivalent to introducing a half magnetic flux with vector potential $A_x = \frac{\pi}{L}$. Treating the response to the vector potential in an analogous fashion to a superconductor, the putative energy cost of an anyon would be

$$\Delta E = \int d^2x \frac{\rho_s}{4} A_x^2 = \rho_s \frac{\pi^2}{4}, \tag{32}$$

where ρ_s is the superfluid stiffness associated with the ground state, $A_x = \pi/L$ is the vector potential, and the factor of 4 derives from halving the energy of the complex fermion system. However, since the complex fermion Hamiltonian H_c preserves the global $U(1)$ symmetry, its superfluid stiffness ρ_s vanishes, so it costs no energy to create anyons in the gapless state. From this line of reasoning, we can see that the ground state of the Kitaev spin liquid has a fourfold degeneracy and is topologically ordered.

The method can also be applied to calculate the energy of visons separated by finite distance by treating the bond flips

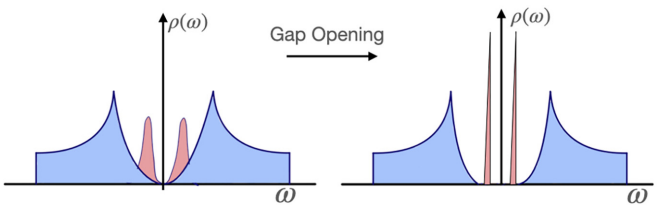

FIG. 5. Schematic illustration of the resonance in the density of states for the gapless Kitaev spin liquid. The resonance becomes sharp when a gap opens in the bulk density of states, forming a fermionic excitation of the vison pair.

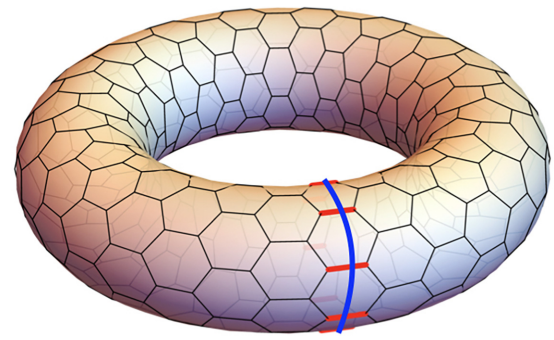

FIG. 6. Hexagonal lattice of Kitaev spin liquid is embedded on a torus by application of the periodic boundary condition. An anyon forms within the torus by flipping the bonds along a noncontractable loop that encircles the torus.

between the two visons as a diffraction problem; however, due to the complex nature of the problem, it is left for future investigation.

Finally, we note that our method also admits various generalizations. For example, it can be extended to anisotropic couplings, i.e., $J_x \neq J_y \neq J_z$, as well as to higher dimensions, such as the three-dimensional hyperoctagonal lattice. Moreover, our method can be applied to study the impact of spinor order formation as a consequence of hybridization between conduction electrons and Majorana spinons in the CPT model for a Kondo lattice coupled to a Yao-Lee spin liquid [27,28]. This allows us to study the stability of the Yao-Lee spin liquid against spinor order formation, which is the subject of a forthcoming article by the authors.

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All authors contributed equally to this work.

APPENDIX A: ANALYTIC CALCULATION OF GREEN'S FUNCTION IN HONEYCOMB LATTICE

Here we show how to simplify the integrals

$$\begin{aligned} g_0(z) &= \int_0^{2\pi} \frac{dk_1}{2\pi} \int_0^{2\pi} \frac{dk_2}{2\pi} \frac{z}{z^2 - |\gamma_{\mathbf{k}}|^2}, \\ g_2(z) &= \int_0^{2\pi} \frac{dk_1}{2\pi} \int_0^{2\pi} \frac{dk_2}{2\pi} \frac{\gamma_c(\mathbf{k})}{z^2 - |\gamma_{\mathbf{k}}|^2}, \end{aligned} \tag{A1}$$

where $\gamma_c(\mathbf{k}) = 1 + \cos(k_1) + \cos(k_2)$, using a contour integral. We begin by noting that the integrals over k_1 and k_2 can be carried out in either order, allowing us to pull the cosines in $\gamma_c(k)$ out of the inner integral, so that

$$\begin{aligned} g_0(z) &= \int_0^{2\pi} \frac{dk_1}{2\pi} z I_0(z, k_1), \\ g_2(z) &= \int_0^{2\pi} \frac{dk_1}{2\pi} (1 + 2\cos k_1) I_0(z, k_1), \end{aligned} \tag{A2}$$

where

$$I_0(z, k) = \int_0^{2\pi} \frac{dk_2}{2\pi} \frac{1}{z^2 - |\gamma_{\mathbf{k}}|^2}. \tag{A3}$$

Writing $s = e^{ik_1}$ and $w = e^{ik_2}$, we can rewrite I_0 as a counterclockwise integral around the unit circle $|w| = 1$,

$$I_0(z, k) \equiv I_0(z, s) = \oint_{|w|=1} \frac{dw}{2\pi i w} \frac{1}{z^2 - |\gamma(s, w)|^2}. \tag{A4}$$

Rewriting the denominator as a quadratic function of w,

$$\begin{aligned} z^2 - |\gamma(s, w)|^2 &= z^2 - (1 + s + w)\left(1 + \frac{1}{s} + \frac{1}{w}\right) \\ &= -\frac{(1+s)}{sw}(w^2 + wb + s), \end{aligned} \tag{A5}$$

where

$$b = \frac{1 + 3s + s^2 - sz^2}{(1+s)}. \tag{A6}$$

We can thus write the integral in the form

$$I_0(z, s) = -\frac{s}{1+s} \oint \frac{dw}{2\pi i} \frac{1}{(w - w_+)(w - w_-)}, \tag{A7}$$

where

$$w_\pm = -\frac{b}{2} \pm \sqrt{\left(\frac{b}{2}\right)^2 - s} \tag{A8}$$

are the poles of the integrand.

Now, since $w_+ w_- = s = e^{ik_1}$, it follows that $|w_+ w_-| = 1$, so that only one of these poles lies inside the contour. [In general, this may depend on the way we treat the branch cuts inside the square root of (A8). However, we do not actually need to know which pole it is, as we will fix the sign and the branch cuts in the final expression by demanding that the asymptotic behavior of $I_0 \sim 1/z^2$ is analytic at large z.] Let us assume that the pole closest to the origin is at $w = w_-$; then we obtain

$$I_0(z, s) = \frac{s}{1+s} \frac{1}{w_+ - w_-} = \frac{s}{1+s} \frac{1}{\sqrt{b^2 - 4s}}. \tag{A9}$$

Now, expanding the denominator, we have

$$\begin{aligned} &(1+s)\sqrt{b^2 - 4s} \\ &= \sqrt{(1 + 3s + s^2 - sz^2)^2 - 4s(1+s)^2} \\ &= s\sqrt{(3 + 2\cos k_1 - z^2)^2 - 8(\cos k + 1)} \\ &= s[z^2 - (3 + 2\cos k_1)]\sqrt{1 - \frac{8(\cos k + 1)}{[z^2 - (3 + 2\cos k_1)]^2}}, \end{aligned} \tag{A10}$$

where we have factorized the final expression to guarantee that, at large z, $I_0(z, s) \sim 1/z^2$ is analytic. Combining the above results gives us the following expressions for $g_0(z)$ and $g_2(z)$:

$$\begin{aligned} g_0(z) &= \int_0^{2\pi} \frac{dk}{2\pi} \frac{z}{[z^2 - (3 + 2c)]\sqrt{1 - \frac{8(c+1)}{[z^2 - (3+2c)]^2}}}, \\ g_2(z) &= \int_0^{2\pi} \frac{dk}{2\pi} \frac{2c + 1}{[z^2 - (3 + 2c)]\sqrt{1 - \frac{8(c+1)}{[z^2 - (3+2c)]^2}}}, \end{aligned} \tag{A11}$$

where $c \equiv \cos(k)$, which are the expressions given in (27) and (28).

APPENDIX B: DENSITY OF SCATTERING STATES AROUND A VISON

In this Appendix we discuss the interpretation of the scattering phase shift in a Majorana scattering problem. For conventional particles, the scattering phase shift is defined in terms of the S matrix, $S = e^{2i\delta}$, associated with the scattering of a partial wave state: what is the appropriate generalization to Majorana excitations? We can answer this question by considering the scattering Hamiltonian. In our problem, the

scattering Hamiltonian is given by (10), which we rewrite in momentum space as

$$\text{KSL}+2v = \frac{1}{2}\sum_{\mathbf{k}\in\mathbf{BZ}} \psi^\dagger_{\mathbf{k}}(\vec{\gamma}_{\mathbf{k}}\cdot\vec{\tau})\psi_{\mathbf{k}} + \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'\in BZ} \psi^\dagger_{\mathbf{k}'}(V\tau_2)\psi_{\mathbf{k}}. \tag{B1}$$

Here the $\psi_{\mathbf{k}}$, which are the Fourier transform of the real-space Majorana fermions, are complex "Dirac" fermions; their underlying Majorana character is enforced by the condition $\psi_{-\mathbf{k}\alpha} = \psi^\dagger_{\mathbf{k}\alpha}$, so that holes formed in one half of the Brillouin zone are equivalent to particles in the other half. This guarantees that the density of states $\rho(E) = \rho(-E)$ is particle-hole symmetric. The factor of $1/2$ in the Hamiltonian avoids overcounting.

An independent set of one-particle excitations can be formed in two ways.

(1) By using all of momentum space, but restricting the excitations exclusively to positive energy, particle excitations; i.e., one-particle eigenstates are

$$|\mathbf{k}\rangle = \sum_\alpha u_{\mathbf{k}\alpha}\psi^\dagger_{\mathbf{k}\alpha}|GS\rangle \quad (\mathbf{k}\in BZ,\ \alpha\in A,B), \tag{B2}$$

where $u_{\mathbf{k}\alpha}\psi^\dagger_{\mathbf{k}\alpha}$ creates a positive energy eigenstate at momentum $\mathbf{k}$. This allows us to discuss the phase shift of scattered, conventional fermions. The density of states is then $N_I(E) = \rho(E)$ and the free energy is given by an integration over positive energy excitations

$$F = -T\int_0^\infty dE\ \ln(1+e^{-\beta E})\rho(E). \tag{B3}$$

(2) Alternatively, restricting $\mathbf{k}$ to one half of the Brillouin zone while considering both particles and holes formed within this half subspace. In this case, the density of states is $N_{II}(E) = \frac{1}{2}\rho(E)$ and the free energy is written

$$\begin{aligned} F &= -\frac{T}{2}\int_{-\infty}^\infty dE\ \ln(1+e^{-\beta E})\rho(E) \\ &= -\frac{T}{2}\int_{-\infty}^\infty dE\ \ln[2\cosh(\beta E/2)]\rho(E), \end{aligned} \tag{B4}$$

where $\rho(E) = \rho(-E)$.

Method (1) is more appropriate for discussing the scattering, while (2) is more aligned with the Green's function approach we have adopted.

To calculate the change in density of states due to the scattering, we note that the change in free energy calculated in (B5),

$$\Delta F = \int_{-\infty}^\infty \frac{d\omega}{2\pi}\left(\frac{1}{2} - f(\omega)\right)\delta_v(\omega), \tag{B5}$$

can be integrated by parts to obtain

$$\Delta F = -\frac{T}{2}\int_0^\infty dE\ \ln\left[2\cosh\frac{\beta E}{2}\right]\left(\frac{1}{\pi}\frac{\partial\delta(E)}{\partial E}\right). \tag{B6}$$

Comparing this with (B3), we see that the change in density of states due to scattering is

$$\delta\rho(E) = \frac{1}{\pi}\frac{\partial\delta(E)}{\partial E}. \tag{B7}$$

We note that this result can also be obtained by observing that the scattering shifts the energy levels E_λ of the continuum downwards by an amount equal to

$$E'_\lambda = E_\lambda - \Delta\frac{\delta(E_\lambda)}{\pi}, \tag{B8}$$

where Δ is the energy spacing of the continuum. The energy spacing is then modified by the scattering to

$$\begin{aligned} \Delta' = E'_{\lambda+1} - E'_\lambda &= \Delta - \frac{\Delta}{\pi}[\delta(E_\lambda+\Delta) - \delta(E_\lambda)] \\ &= \Delta\left[1 - \frac{\Delta}{\pi}\frac{\partial\delta}{\partial E}\right]. \end{aligned} \tag{B9}$$

If the original density of states is $\frac{1}{\Delta} = \rho(E)$, the modified density of states is then

$$\begin{aligned} \rho(E) + \delta\rho(E) = \frac{1}{\Delta'} &= \frac{1}{\Delta}\left[1 - \frac{\Delta}{\pi}\frac{\partial\delta}{\partial E}\right]^{-1} \\ &= \rho(E) + \frac{1}{\pi}\frac{\partial\delta(E)}{\partial E}, \end{aligned} \tag{B10}$$

so that the change in the density of states is given by

$$\Delta\rho(E) = \frac{1}{\pi}\frac{\partial\delta(E)}{\partial E}. \tag{B11}$$

[1] A. Kitaev, Ann. Phys. (NY) **321**, 2 (2006).

[2] M. Hermanns, I. Kimchi, and J. Knolle, Annu. Rev. Condens. Matter Phys. **9**, 17 (2018).

[3] K. O'Brien, M. Hermanns, and S. Trebst, Phys. Rev. B **93**, 085101 (2016).

[4] S. Trebst and C. Hickey, Phys. Reports **950**, 1 (2022).

[5] H. Takagi, T. Takayama, G. Jackeli, G. Khaliullin, and S. E. Nagler, Nat. Rev. Phys. **1**, 264 (2019).

[6] A. Banerjee, C. A. Bridges, J.-Q. Yan, A. A. Aczel, L. Li, M. B. Stone, G. E. Granroth, M. D. Lumsden, Y. Yiu, J. Knolle, S. Bhattacharjee, D. L. Kovrizhin, R. Moessner, D. A. Tennant, D. G. Mandrus, and S. E. Nagler, Nat. Mater. **15**, 733 (2016).

[7] S.-H. Do, S.-Y. Park, J. Yoshitake, J. Nasu, Y. Motome, Y. Kwon, D. T. Adroja, D. J. Voneshen, K. Kim, T.-H. Jang, J.-H. Park, K.-Y. Choi, and S. Ji, Nat. Phys. **13**, 1079 (2017).

[8] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. **102**, 017205 (2009).

[9] Y. Kasahara, T. Ohnishi, Y. Mizukami, O. Tanaka, S. Ma, K. Sugii, N. Kurita, H. Tanaka, J. Nasu, Y. Motome, T. Shibauchi, and Y. Matsuda, Nature (London) **559**, 227 (2018).

[10] H. Liu, J. Chaloupka, and G. Khaliullin, Phys. Rev. Lett. **125**, 047201 (2020).

[11] S. M. Winter, A. A. Tsirlin, M. Daghofer, J. van den Brink, Y. Singh, P. Gegenwart, and R. Valentí, J. Phys.: Condens. Matter **29**, 493002 (2017).

[12] A. U. B. Wolter, L. T. Corredor, L. Janssen, K. Nenkov, S. Schoönecker, S.-H. Do, K.-Y. Choi, R. Albrecht, J. Hunger,

T. Doert, M. Vojta, and B. Buüchner, Phys. Rev. B **96**, 041405(R) (2017).
[13] D. Wulferding, Y. Choi, S.-H. Do, C. H. Lee, P. Lemmens, C. Faugeras, Y. Gallais, and K.-Y. Choi, Nat. Commun. **11**, 1603 (2020).
[14] M. G. Yamada, npj Quantum Mater. **5**, 82 (2020).
[15] J. Chaloupka, G. Jackeli, and G. Khaliullin, Phys. Rev. Lett. **105**, 027204 (2010).
[16] K. Kitagawa, T. Takayama, Y. Matsumoto, A. Kato, R. Takano, Y. Kishimoto, S. Bette, R. Dinnebier, G. Jackeli, and H. Takagi, Nature (London) **554**, 341 (2018).
[17] T. Eschmann, P. A. Mishchenko, T. A. Bojesen, Y. Kato, M. Hermanns, Y. Motome, and S. Trebst, Phys. Rev. Res. **1**, 032011(R) (2019).
[18] K. Feng, N. B. Perkins, and F. J. Burnell, Phys. Rev. B **102**, 224402 (2020).
[19] A. P. Joy and A. Rosch, Phys. Rev. X **12**, 041004 (2022).
[20] Y. Kato, Y. Kamiya, J. Nasu, and Y. Motome, Phys. Rev. B **96**, 174409 (2017).
[21] H. Li, D.-W. Qu, H.-K. Zhang, Y.-Z. Jia, S.-S. Gong, Y. Qi, and W. Li, Phys. Rev. Res. **2**, 043015 (2020).
[22] J. Nasu, M. Udagawa, and Y. Motome, Phys. Rev. B **92**, 115122 (2015).
[23] Y. Motome and J. Nasu, J. Phys. Soc. Jpn. **89**, 012002 (2020).
[24] M. Udagawa and R. Moessner, arXiv:1912.01545.
[25] H. Yao and S. A. Kivelson, Phys. Rev. Lett. **99**, 247203 (2007).
[26] H. Yao and D.-H. Lee, Phys. Rev. Lett. **107**, 087205 (2011).
[27] P. Coleman, A. Panigrahi, and A. Tsvelik, Phys. Rev. Lett. **129**, 177601 (2022).
[28] A. M. Tsvelik and P. Coleman, Phys. Rev. B **106**, 125144 (2022).
[29] G. Baskaran, S. Mandal, and R. Shankar, Phys. Rev. Lett. **98**, 247201 (2007).
[30] J. Knolle, D. L. Kovrizhin, J. T. Chalker, and R. Moessner, Phys. Rev. Lett. **112**, 207203 (2014).
[31] V. Lahtinen, New J. Phys. **13**, 075009 (2011).
[32] V. Lahtinen, A. W. W. Ludwig, and S. Trebst, Phys. Rev. B **89**, 085121 (2014).
[33] V. Lahtinen, G. Kells, A. Carollo, T. Stitt, J. Vala, and J. K. Pachos, Ann. Phys. (NY) **323**, 2286 (2008).
[34] V. Lahtinen, A. W. W. Ludwig, J. K. Pachos, and S. Trebst, Phys. Rev. B **86**, 075115 (2012).
[35] H. Théveniaut and M. Vojta, Phys. Rev. B **96**, 054401 (2017).
[36] W.-H. Kao, J. Knolle, G. B. Halász, R. Moessner, and N. B. Perkins, Phys. Rev. X **11**, 011034 (2021).
[37] S.-S. Zhang, Z. Wang, G. B. Halász, and C. D. Batista, Phys. Rev. Lett. **123**, 057201 (2019).
[38] E. H. Lieb, Phys. Rev. Lett. **73**, 2158 (1994).
[39] F. D. M. Haldane, Phys. Rev. Lett. **61**, 2015 (1988).