SUPPLEMENTAL MATERIAL: Characterization of topological states via dual multipartite entanglement

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I. MAPPING TO THE EXTENDED ISING MODEL AND EXACT SOLUTIONS

We start from the extended quantum Ising model with longer-range interactions in a transverse field, with the Hamiltonian

$$H=\sum_{n=1}^{N_f}\sum_{j=1}^{L}\left(\frac{J_n^x}{2}\sigma_j^x\sigma_{j+n}^x+\frac{J_n^y}{2}\sigma_j^y\sigma_{j+n}^y\right)\prod_{l=j+1}^{j+n-1}\sigma_l^z+\sum_{j=1}^{L}\frac{\mu}{2}\sigma_j^z, \tag{S1}$$

where $\sigma_j^{x,y,z}$ are Pauli matrices for the spin at site j, and L (assumed even) is the total number of sites. By the Jordan-Wigner transformation

$$c_1=-\sigma_1^+=-(\sigma_1^x+i\sigma_1^y)/2,\qquad c_j=-\sigma_j^+\prod_{i=1}^{j-1}\sigma_i^z, \tag{S2}$$

we can obtain a spinless fermion Hamiltonian with longer-range pairing and hopping terms with fermion parity $(-1)^{N_p}$ of the number of fermions

$$N_p=\sum_{j=1}^{L}c_j^\dagger c_j, \tag{S3}$$

as $H=H_o+H_b$, where the open chain part is

$$\begin{aligned}H_o=&\sum_{n=1}^{N_f}\sum_{j=1}^{L-n}\left(\frac{J_n^+}{2}c_j^\dagger c_{j+n}+\frac{J_n^-}{2}c_j^\dagger c_{j+n}^\dagger+\text{h.c.}\right)\\&-\sum_{j=1}^{L}\mu\left(c_j^\dagger c_j-\frac{1}{2}\right),\end{aligned} \tag{S4}$$

and the boundary part reads

$$H_b=\frac{(-1)^{N_p}}{2}\sum_{n=1}^{N_f}\sum_{j=L-n+1}^{L}(J_n^+c_j^\dagger c_{j+n}+J_n^-c_j^\dagger c_{j+n}^\dagger+\text{h.c.}), \tag{S5}$$

with $J_n^\pm\equiv J_n^x\pm J_n^y$. Thus, given a definite even fermion parity $(-1)^{N_p}=1$, this extended Kitaev fermion chain [1] has an antiperiodic boundary condition $c_{j+L}=-c_j$. Here we choose all the hopping and pairing parameters as real, which make the Hamiltonian preserve time-reversal symmetry and belong to the BDI class (**Z** type) characterized by the winding numbers [2, 3].

For the thermodynamic limit $L\gg N_f\geq 1$, we use the Fourier transformation,

$$c_j=\frac{1}{\sqrt{L}}\sum_q\exp(-iqj)\,c_q, \tag{S6}$$

to express the Bogoliubov-de Gennes Hamiltonian as

$$H=\sum_q(c_q^\dagger,c_{-q})\mathcal{H}_q\begin{pmatrix}c_q\\c_{-q}^\dagger\end{pmatrix}, \tag{S7}$$

where the complete set of wavevectors is $q=2\pi m/L$ with

$$m=-\frac{L-1}{2},-\frac{L-3}{2},\cdots,\frac{L-3}{2},\frac{L-1}{2}. \tag{S8}$$

Here, we can write

$$\mathcal{H}_q=\frac{1}{2}\boldsymbol{r}(q)\cdot\boldsymbol{\sigma}, \tag{S9}$$

with the vector $\boldsymbol{r}(q)=(0,y(q),z(q))$ in the auxiliary two-dimensional y-z space,

$$y(q)=\sum_{n=1}^{N_f}J_n^-\sin(nq), \tag{S10}$$

$$z(q)=\sum_{n=1}^{N_f}J_n^+\cos(nq)-\mu, \tag{S11}$$

and $\boldsymbol{\sigma}=(\sigma^x,\sigma^y,\sigma^z)$. Using the Bogoliubov transformation

$$c_q=\cos\frac{\Theta}{2}\eta_q+i\sin\frac{\Theta}{2}\eta_{-q}^\dagger, \tag{S12}$$

with $\tan\Theta=y(q)/z(q)$, we can diagonalize the Hamiltonian as

$$H=\sum_q\epsilon_q\left(\eta_q^\dagger\eta_q-\frac{1}{2}\right), \tag{S13}$$

and obtain the ground state

$$|\mathcal{G}\rangle=\prod_q[\cos\frac{\Theta}{2}+i\sin\frac{\Theta}{2}\eta_q^\dagger\eta_{-q}^\dagger]|0\rangle, \tag{S14}$$

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where the energy spectra are

$$\epsilon_q = \pm\frac{1}{2}\sqrt{y(q)^2 + z(q)^2}. \tag{S15}$$

In Fig. S1, we plot the energy spectra for $L = 200$ and trajectories of winding vectors for four different extended Kitaev fermion chain models [1] considered in the main text.

II. WINDING NUMBERS

For the BDI symmetry class Kitaev chain fermion systems, the winding number in the auxiliary space of momentum behaves as a $\mathbf{Z}$ topological invariant [2, 4], which is a fundamental concept in geometric topology. The winding number of the closed loop in auxiliary y-z plane around the origin can be written as

$$\nu = \frac{1}{2\pi}\oint \frac{ydz - zdy}{|\boldsymbol{r}|^2}. \tag{S16}$$

Via the substitution $\zeta(q) \equiv \exp(iq)$, we can rewrite in complex space that

$$y(q) = \sum_{n=1}^{N_f} \frac{J_n^-(\zeta^n - \zeta^{-n})}{2i} \equiv Y(\zeta), \tag{S17}$$

and

$$z(q) = \sum_{n=1}^{N_f} \frac{J_n^+(\zeta^n + \zeta^{-n})}{2} - \mu \equiv Z(\zeta). \tag{S18}$$

By defining a complex characteristic function

$$g(\zeta) \equiv Z(\zeta) + iY(\zeta) \tag{S19}$$

$$= \sum_{n=1}^{N_f}(J_n^x\zeta^n + J_n^y\zeta^{-n}) - \mu, \tag{S20}$$

we obtain the winding number by calculating the logarithmic residue of $g(\zeta)$ in accordance with the Cauchy's argument principle [5]

$$\nu = \frac{1}{2\pi i}\oint_{|\zeta|=1} d\zeta\,\frac{g'(\zeta)}{g(\zeta)} = \mathcal{N} - \mathcal{P}, \tag{S21}$$

where in the complex region $|\zeta| < 1$, $\mathcal{N}$ is the number of zeros for $g(\zeta) = 0$, and $\mathcal{P}$ is the number of poles for $g(\zeta) = \infty$. For two special cases: $J_n^y = 0\ \forall n$, we have

$$g(\zeta) = \sum_{n=1}^{N_f} J_n^x\zeta^n + \mu, \tag{S22}$$

and only zeros exist; while $J_n^x = 0$ there only poles exist.

III. MAJORANA ZERO MODES

We can write the open-chain Hamiltonian (S4) in terms of Majorana fermion operators:

$$a_j = c_j^\dagger + c_j, \qquad b_j = i(c_j^\dagger - c_j), \tag{S23}$$

with relations $\{a_i, a_j\} = \{b_i, b_j\} = 2\delta_{ij}$, $\{a_i, b_j\} = 0$ as

$$H_o = -\frac{i}{2}\sum_{n=1}^{N_f}\sum_{j=1}^{L-n}(J_n^x b_j a_{j+n} + J_n^y b_{j+n} a_j) + \frac{i\mu}{2}\sum_{j=1}^{L} a_j b_j. \tag{S24}$$

We can assume an ansatz wave function as a linear combination of Majorana operators a_j [6]:

$$\phi = \sum_{j=1}^{L}\alpha_j a_j, \tag{S25}$$

and calculate the commutation to satisfy the condition $[H, \phi] = 0$ for the existence of Majorana zero modes [7, 8]. Then, the coefficients are given by the recursion relations

$$\sum_{n=1}^{N_f}(J_n^x\alpha_{j+n} + J_n^y\alpha_{j-n}) - \mu\alpha_j = 0, \tag{S26}$$

for $j = n+1, n+2\cdots, L-n$. These recursion equations can be solved with the solutions of characteristic equations $g(\zeta) = 0$ [9] given $g(\zeta)$ in Eq. (S20). If $\mathcal{N} \geq \mathcal{P}$, we should require Majorana zero modes at the left end satisfying $|\alpha_L| \to 0$, for the thermodynamic limit $L \gg 1$, and only in the range $|\zeta| < 1$ should the zeros $\{\zeta_l\}$ be considered. Thus, we have $\mathcal{N}$ independent solutions

$$\alpha_j = \sum_{l=1}^{\mathcal{N}}\omega_l(\zeta_l)^j, \tag{S27}$$

with $\{\omega_l\}$ undetermined coefficients, and for $j \leq \mathcal{P}$, we have $\mathcal{P}$ constraint conditions

$$\sum_{n=1}^{N_f} J_n^x\alpha_{j+n} + \mu\alpha_j + \sum_{n=1}^{j-1} J_n^y\alpha_{j-n} = 0. \tag{S28}$$

Thus, we have $(\mathcal{N} - \mathcal{P})$ independent normalized left zero modes $\phi_{\mathrm{L}}^1, ..., \phi_{\mathrm{L}}^{(\mathcal{N}-\mathcal{P})}$ with coefficients $\{\alpha_j^1\}, ..., \{\alpha_j^{(\mathcal{N}-\mathcal{P})}\}$, where the orthogonal Majorana zero modes can be obtained by using the Schmidt orthogonalization with conditions $\{\phi^i, \phi^{j\dagger}\} = 2\delta_{ij}$. These considerations also hold for linear combinations of Majorana operators $\{b_j\}$ with the form

$$\psi^i = \sum_{j=1}^{L}\beta_j^i b_j, \tag{S29}$$

and

$$\beta_j^i = \alpha_{L-j+1}^i, \tag{S30}$$

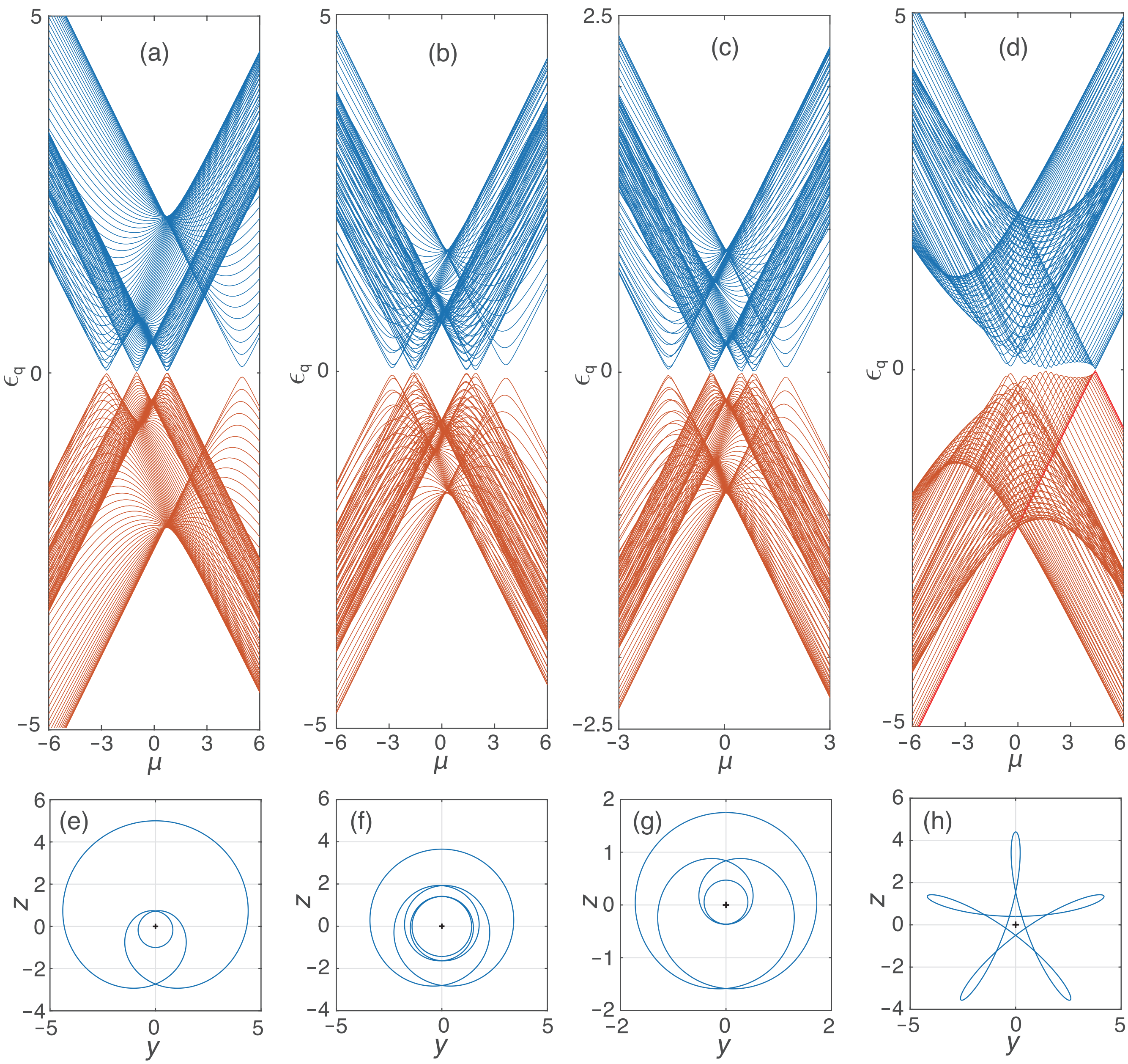

FIG. S1. (color online) (a-d) Energy spectra for $L = 200$ and (e-h) trajectories of winding vectors for an extended Kitaev fermion chain with parameters: (a,e) $J_1^+ = J_1^- = 1$, $J_2^+ = J_2^- = 2$, $J_3^+ = J_3^- = 2$ ($N_f = 3$); (b,f) $J_1^+ = J_1^- = 0.1$, $J_2^+ = J_2^- = 0.21$, $J_3^+ = J_3^- = 0.44$, $J_4^+ = J_4^- = 0.9$, $J_5^+ = J_5^- = 2$ ($N_f = 5$); (c,g) $J_1^+ = J_1^- = 0.1$, $J_2^+ = J_2^- = 0.21$, $J_3^+ = J_3^- = -0.74$, $J_4^+ = J_4^- = 0.9$ ($N_f = 4$); and (d,h) $J_2^+ = J_2^- = 2.4$, $J_3^+ = 2$, $J_3^- = -2$ ($N_f = 3$).

because Majorana zero modes appear in pairs [10]. For the other case $\mathcal{N} < \mathcal{P}$, we should consider right Majorana zero modes that require $|\alpha_1| \to 0$ for $L \gg 1$ and the characteristic equation $\bar{g}(\zeta) = g(1/\zeta) = 0$, with $\bar{\mathcal{N}}$ zeros and $\bar{\mathcal{P}}$ poles in $|\zeta| < 1$, where we can obtain that

$$\mathcal{N} + \bar{\mathcal{N}} = \bar{\mathcal{P}} + \mathcal{P}, \tag{S31}$$

and have $(\mathcal{P} - \mathcal{N})$ right Majorana zero modes $\phi_{\mathrm{R}}^1, \phi_{\mathrm{R}}^2, \cdots, \phi_{\mathrm{R}}^{(\mathcal{P}-\mathcal{N})}$. Therefore, we derive that in the thermodynamic limit $L \gg N_f \geq 1$, the number of Majorana zero modes at each end of the extended Kitaev open chain, defined as $\mathcal{M}_0$, equals the absolute value of the winding number:

$$\mathcal{M}_0 = |\mathcal{N} - \mathcal{P}| = |\nu|. \tag{S32}$$

Here, we should note that there exist special cases when degenerate solutions of Majorana zero modes might occur for some choices of parameters and could be averted as we consider the perturbation of characteristic functions.

Moreover, while the coefficients $\{\alpha_j\}$ are not real, the zero modes ϕ and ψ, with conditions $\{\phi^i, {\phi^j}^\dagger\} = \{\psi^i, {\psi^j}^\dagger\} = 2\delta_{ij}$ and $\{\phi^i, {\psi^j}^\dagger\} = \{\phi^i, \psi^j\} = 0$, are not Majorana operators [11]. Fortunately, for $\mathcal{N} \geq \mathcal{P}$, left and right Majorana zero modes can be combined as $(\mathcal{N} - \mathcal{P})$ fermion modes $d^1, d^2, \cdots, d^{(\mathcal{N}-\mathcal{P})}$ with

$$d^i = (\phi^i_{\rm L} + i\psi^i_{\rm R})/2, \tag{S33}$$

that commute with the Hamiltonian in the thermodynamic limit. Conversely, for $\mathcal{P} \geq \mathcal{N}$, there exist $(\mathcal{P} - \mathcal{N})$ fermion zero modes with operators $\bar{d}^1, \bar{d}^2, \cdots, \bar{d}^{(\mathcal{P}-\mathcal{N})}$, where

$$\bar{d}^i = (\phi^i_{\rm R} + i\psi^i_{\rm L})/2. \tag{S34}$$

Our discussions also provide an effective method for finding the distribution of Majorana zero modes by finding the zeros and poles of the characteristic functions $g(\zeta)$ in momentum space. Moreover, the topological phase transitions occur when the parameters satisfy the existence of zeros of the characteristic functions on the critical contour $|\zeta| = 1$, see Sec. VII for details.

IV. QUANTUM FISHER INFORMATION OF TOPOLOGICAL STATES

Given a generator $\mathcal{O}$ with respect to the parameter t, the quantum Fisher information of the pure ground state $|\mathcal{G}\rangle$ can be written as [12–15]

$$F_Q[\mathcal{O}, |\mathcal{G}\rangle] \;=\; 4(\Delta\mathcal{O})^2 \;=\; 4(\langle\mathcal{O}^2\rangle_{\mathcal{G}} - \langle\mathcal{O}\rangle^2_{\mathcal{G}}). \tag{S35}$$

For critical systems with L sites, we consider the quantum Fisher information density with the form

$$f_Q[\mathcal{O}, |\mathcal{G}\rangle] = \frac{F_Q[\mathcal{O}, |\mathcal{G}\rangle]}{L}, \tag{S36}$$

and the violation of the inequality $f_Q \leq \kappa$ signals $(\kappa+1)$-partite entanglement $(1 \leq \kappa \leq L-1)$.

For instance, we consider a Kitaev chain which is a tight-binding model with strengths of tunneling J and superconducting pairing Δ [10]:

$$H = \sum_{j=1}^{L-1}\left(\frac{\Delta}{2}c_j c_{j+1} - \frac{J}{2}c_j^\dagger c_{j+1} + \text{h.c.}\right) - \mu\sum_{j=1}^{L}\left(n_j - \frac{1}{2}\right), \tag{S37}$$

with the fermion number operator $n_j \equiv c_j^\dagger c_j$. For $J = \Delta$ and zero chemical potentials $\mu = 0$, we have one Majorana zero mode at each end, and the Hamiltonian may be written in terms of Majorana operators and Dirac fermion operators

$$d_{j,1} = (b_j + i a_{j+1})/2 \tag{S38}$$

as a diagonal form

$$H = i\frac{J}{2}\sum_{j=1}^{L-1} b_j a_{j+1} = \sum_{j=1}^{L-1} J\left(d_{j,1}^\dagger d_{j,1} - \frac{1}{2}\right), \tag{S39}$$

where we have a winding number $\nu = 1$. Here, to detect multipartite entanglement, it requires to choose a pair of nonlocal generators [16]

$$\mathcal{O}_{\nu=1} = \sum_{j=1}^{L}\sigma_j^x/2, \qquad \mathcal{O}^{(\rm st)}_{\nu=1} = \sum_{j=1}^{L}(-)^j\sigma_j^x/2. \tag{S40}$$

Using the Jordan-Wigner transformation as

$$-\sigma_j^x = c_j^\dagger \exp\left(i\pi\sum_{l=1}^{j-l} c_l^\dagger c_l\right) + \exp\left(-i\pi\sum_{l=1}^{j-l} c_l^\dagger c_l\right) c_j, \tag{S41}$$

the quantum Fisher information density of the ground state of the Kitaev chain can be written in terms of longitudinal spin-spin correlation functions:

$$f_Q[\mathcal{O}_{\nu=1}, |\mathcal{G}\rangle] = 1 + \sum_{r=1}^{L-1} C_{\nu=1}(r), \tag{S42}$$

$$f_Q[\mathcal{O}^{(\rm st)}_{\nu=1}, |\mathcal{G}\rangle] = 1 + \sum_{r=1}^{L-1}(-)^r C_{\nu=1}(r), \tag{S43}$$

with respect to the generators $\mathcal{O}_{\nu=1}$ and $\mathcal{O}^{(\rm st)}_{\nu=1}$, respectively. Here, we have used the fact that $\langle\sigma_j^x\rangle_{\mathcal{G}} = 0$ and considered a closed chain for $L \gg 1$. Moreover, the x-directional longitudinal correlation function can be written as

$$C_{\nu=1}(r) = \left\langle\prod_{l=i}^{j-1}(-ib_l a_{l+1})\right\rangle_{\mathcal{G}} = \left\langle\prod_{l=i}^{j-1}(1 - 2d_{l,1}^\dagger d_{l,1})\right\rangle_{\mathcal{G}}, \tag{S44}$$

which represents the average of the Majorana parity from site i to j $(j - i = r)$ and does not include the edge modes. For $J > 0$, we have

$$\langle d_{l,1}^\dagger d_{l,1}\rangle_{\mathcal{G}} = 0, \tag{S45}$$

so the Majorana zero modes give

$$f_Q[\mathcal{O}_{\nu=1}, |\mathcal{G}\rangle] = L, \tag{S46}$$

which signals the maximal L-partite entanglement with the generator $\mathcal{O}_{\nu=1}$. On the contrary, for $J < 0$, we have

$$\langle d_{l,1}^\dagger d_{l,1}\rangle_{\mathcal{G}} = 1, \tag{S47}$$

such that the edge Majorana zero modes lead to the fact that

$$f_Q[\mathcal{O}^{(\rm st)}_{\nu=1}, |\mathcal{G}\rangle] = L, \tag{S48}$$

with respect to the generator $\mathcal{O}^{(\rm st)}_{\nu=1}$. Therefore, the choice of generators between the operator $\mathcal{O}_{\nu=1}$ and the staggered operator $\mathcal{O}^{(\rm st)}_{\nu=1}$ depends on the sign of the direct interaction between the chain ends as discussed in Ref. [10]. These results also hold for the open chain, because the correlation function does not include the fermion edge modes. For the other case, we choose $J = -\Delta$ and $\mu = 0$, where the winding number is

$\nu = -1$. Then, the quantum Fisher information density f_Q of the ground state $|\mathcal{G}\rangle$ with respect to the generators:

$$\mathcal{O}_{\nu=-1} = \sum_{j=1}^{L} \sigma_j^y/2, \qquad \mathcal{O}_{\nu=-1}^{(\mathrm{st})} = \sum_{j=1}^{L} (-)^j \sigma_j^y/2. \quad \text{(S49)}$$

can detect symmetry-protected topological order and Majorana zero modes with $\nu = -1$.

The interchange between the quantum phases with positive and negative winding numbers $\nu = \pm 1$

$$\mathcal{O}_{\nu=1}^{(\mathrm{st})} \leftrightarrow \mathcal{O}_{\nu=-1}^{(\mathrm{st})}, \qquad \mathcal{O}_{\nu=1} \leftrightarrow \mathcal{O}_{\nu=-1} \quad \text{(S50)}$$

$$f_Q[\mathcal{O}_{\nu=1}^{(\mathrm{st})}] \leftrightarrow f_Q[\mathcal{O}_{\nu=-1}^{(\mathrm{st})}], \qquad f_Q[\mathcal{O}_{\nu=1}] \leftrightarrow f_Q[\mathcal{O}_{\nu=-1}] \quad \text{(S51)}$$

can be realized by a phase redefinition $c_j \to \pm i c_j$. Another interchange between the staggered operator $\mathcal{O}_{\nu=1}^{(\mathrm{st})}$ and the operator $\mathcal{O}_{\nu=1}$, for the positive and negative signs of the interaction between Dirac fermions localized at the chain ends, respectively,

$$\mathcal{O}_{\nu=1}^{(\mathrm{st})} \leftrightarrow \mathcal{O}_{\nu=1}, \qquad \mathcal{O}_{\nu=-1}^{(\mathrm{st})} \leftrightarrow \mathcal{O}_{\nu=-1} \quad \text{(S52)}$$

$$f_Q[\mathcal{O}_{\nu=1}^{(\mathrm{st})}] \leftrightarrow f_Q[\mathcal{O}_{\nu=1}], \qquad f_Q[\mathcal{O}_{\nu=-1}^{(\mathrm{st})}] \leftrightarrow f_Q[\mathcal{O}_{\nu=-1}] \quad \text{(S53)}$$

can be realized by a Hermitian conjugate transformation $c_j \to c_j^\dagger$.

Generally for $\mu \neq 0$, we can calculate the longitudinal correlation function by defining

$$A_l = c_l^\dagger + c_l = a_l, \qquad B_l = c_l^\dagger - c_l = -i b_l. \quad \text{(S54)}$$

The correlation functions in the x and y directions can be written as

$$C_{\nu=1}(r) = \langle \mathcal{G} | B_i A_{i+1} ... A_{j-1} B_{j-1} A_j | \mathcal{G} \rangle, \quad \text{(S55)}$$

$$C_{\nu=-1}(r) = -\langle \mathcal{G} | A_i B_{i+1} ... B_{j-1} A_{j-1} B_j | \mathcal{G} \rangle, \quad \text{(S56)}$$

where $j - i = r$. Using Wick's theorem, we can write the x-directional spin correlation function into a determinant of size r [17]

$$C_{\nu=1}(r) = \begin{vmatrix} G_{-1} & G_{-2} & \cdots & G_{-r} \\ G_0 & G_{-1} & \cdots & G_{-r+1} \\ G_1 & G_0 & \cdots & G_{-r+2} \\ \vdots & \vdots & \vdots & \vdots \\ G_{r-2} & G_{r-3} & \cdots & G_{-1} \end{vmatrix}, \quad \text{(S57)}$$

and similarly, we have the y-directional spin correlation function as

$$C_{\nu=-1}(r) = \begin{vmatrix} G_1 & G_0 & \cdots & G_{-r+2} \\ G_2 & G_1 & \cdots & G_{-r+3} \\ G_3 & G_2 & \cdots & G_{-r+4} \\ \vdots & \vdots & \vdots & \vdots \\ G_r & G_{r-1} & \cdots & G_1 \end{vmatrix}, \quad \text{(S58)}$$

where we have

$$G_{-r} \equiv \langle \mathcal{G} | B_i A_{i+r} | \mathcal{G} \rangle \quad \text{(S59)}$$

and $\langle \mathcal{G} | A_i A_j | \mathcal{G} \rangle = \langle \mathcal{G} | B_i B_j | \mathcal{G} \rangle = \delta_{ij}$.

V. DUALITY TRANSFORMATION

The duality transformation connects different but equivalent mathematical descriptions of a system or a state of matter through a mapping by the change of variables in quantum physics [18–21]. For example, an Ising chain with an external field h has a self-duality symmetry, mapping between the ordered and disordered phases, expressed as

$$H_{\mathrm{Ising}} = \sum_j (\sigma_j^x \sigma_{j+1}^x + h \sigma_j^z) = h \sum_j (s_j^x s_{j+1}^x + h^{-1} s_j^z) \quad \text{(S60)}$$

with the duality transformation

$$s_j^x = \prod_{k \leq j} \sigma_k^z, \qquad s_j^z = \sigma_j^x \sigma_{j+1}^x, \qquad s_j^y = -i s_j^z s_j^x, \quad \text{(S61)}$$

where both σ and s satisfy the same algebra. By this duality transformation, the cluster Ising model [19, 22] can be mapped to an anisotropic XY model

$$H_{\mathrm{cluster}} = \sum_j (\sigma_{j-1}^x \sigma_j^z \sigma_{j+1}^x + h \sigma_j^z) \quad \text{(S62)}$$

$$= \sum_j (-s_j^y s_{j+1}^y + h s_j^x s_{j+1}^x), \quad \text{(S63)}$$

of which the ordered phase can help to characterize the symmetry-protected topological phase by a $\mathbf{Z}_2 \times \mathbf{Z}_2$ symmetry of the cluster Ising model. Therefore, as shown in [19, 22], this symmetry-protected topological phase can be characterized by the *unlocal* string correlation function [23] equal to a *local* correlator in the dual lattice of the Ising model with the form

$$(-)^r C_{\nu=2}(r) = (-)^r \langle s_j^y s_{j+r}^y \rangle_{\mathcal{G}} \quad \text{(S64)}$$

$$= (-)^r \left\langle \sigma_j^x \sigma_{j+1}^y \left(\prod_{k=2}^{r-1} \sigma_{j+k}^z \right) \sigma_{j+r}^y \sigma_{j+r+1}^x \right\rangle_{\mathcal{G}}, \quad \text{(S65)}$$

from site j to $(j + r)$ in the dual lattice. It is shown in Ref. [24] that the Jordan-Wigner transformation mapping between a one-dimensional spin-$\frac{1}{2}$ model and free fermion chain can also be regarded as a dual transformation with a bond-algebraic approach. Through the Jordan-Wigner transformation, the cluster Ising model corresponds to an extended Kitaev chain with a $\mathbf{Z}_4$ symmetry. Thus, the self-duality properties of the Ising model (S63) can help to study topological phases and multipartite entanglement in the symmetry-protected phase with a winding number $\nu = 2$ in the extended Kitaev chain. Generally, we find that for the extended Kitaev chain, the string correlation function can be written as a spin correlation function with respect to the spin operators from the self-duality symmetry of the extended Ising model.

The duality transformation for topological phases with a

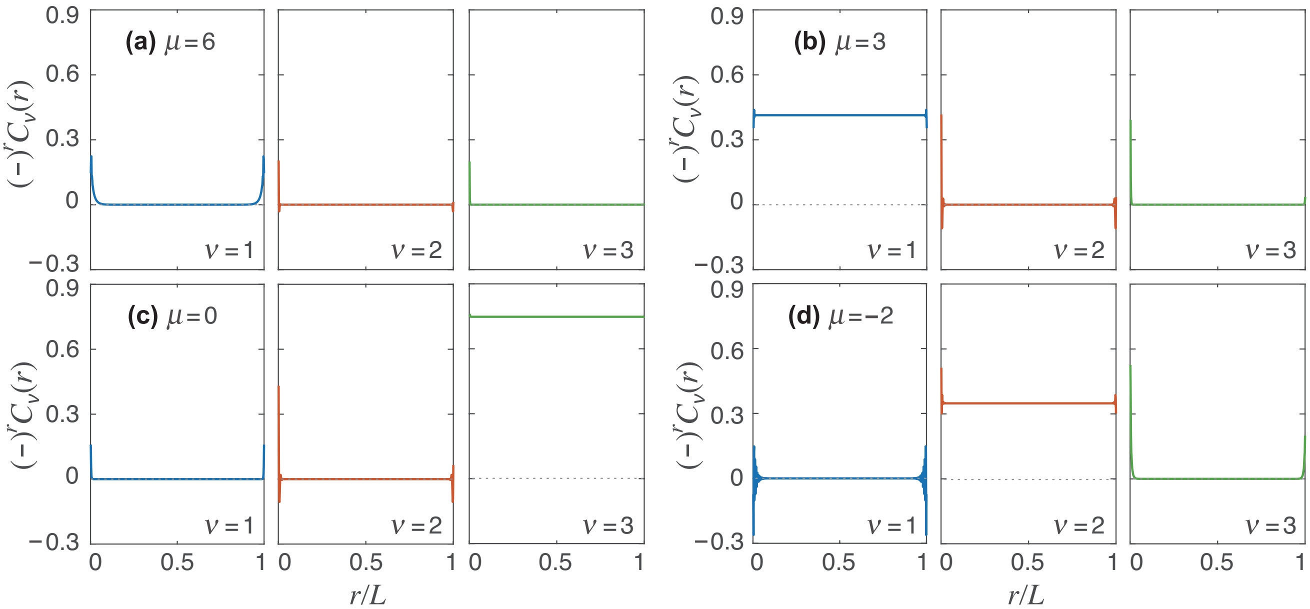

FIG. S2. (color online) The staggered string correlation functions $(-)^r C_\nu(r)$ versus the normalized distance r/L for the extended Kitaev fermion chain with a system size $L = 600$, third neighbor interactions ($N_f = 3$) and nonzero parameters: $J_1^+ = J_1^- = 1$, $J_2^+ = J_2^- = 2$, $J_3^+ = J_3^- = 2$.

μ	$\lambda^{(\mathrm{st})}_{\nu=1}$	$\lambda_{\nu=1}$	$\lambda^{(\mathrm{st})}_{\nu=2}$	$\lambda_{\nu=2}$	$\lambda^{(\mathrm{st})}_{\nu=3}$	$\lambda_{\nu=3}$	$\lambda^{(\mathrm{st})}_{\nu=4}$	$\lambda_{\nu=4}$
1	4.8×10^{-7}	0.9837	-2.0×10^{-6}	2.1×10^{-6}	-8.0×10^{-7}	4.4×10^{-5}	1.9×10^{-6}	5.2×10^{-7}
0.6	-8.6×10^{-8}	8.0×10^{-8}	-1.3×10^{-7}	3.3×10^{-8}	-6.9×10^{-8}	0.9941	7.4×10^{-7}	-3.5×10^{-8}
0	5.8×10^{-14}	-6.7×10^{-14}	3.1×10^{-14}	1.5×10^{-14}	6.1×10^{-14}	-5.5×10^{-14}	1.0051	2.5×10^{-13}
−1	9.5×10^{-14}	-2.4×10^{-13}	0.9933	2.1×10^{-14}	-2.2×10^{-14}	-1.6×10^{-13}	3.3×10^{-14}	3.8×10^{-14}

TABLE I. Fitting of the scaling coefficients λ_ν and $\lambda_\nu^{(\mathrm{st})}$ with respect to the dual generators $\mathcal{O}_\nu$ and $\mathcal{O}_\nu^{(\mathrm{st})}$, respectively, for the different topological phases for the extended Kitaev fermion chain with parameters $J_1^+ = J_1^- = 0.1$, $J_2^+ = J_2^- = 0.21$, $J_3^+ = J_3^- = -0.74$, $J_4^+ = J_4^- = 0.9$ ($N_f = 4$), and chain length up to $L = 2000$. The four essentially non-zero scaling coefficients are shown in blue font, and all four are close to 1.

winding number $\nu = 2$ can be written as

$$\mathbb{Z}_j^{(2)} = \sigma_j^x \sigma_{j+1}^x, \qquad \mathbb{X}_j^{(2)} = \prod_{l=1}^{j} \sigma_l^z, \tag{S66}$$

$$\mathbb{Y}_j^{(2)} = -i\mathbb{Z}_j^{(2)}\mathbb{X}_j^{(2)} = -\left(\prod_{l=1}^{j-1} \sigma_l^z\right) \sigma_j^y \sigma_{j+1}^x \tag{S67}$$

which implies that

$$\mathbb{X}_j^{(2)}\mathbb{X}_{j+1}^{(2)} = \sigma_{j+1}^z. \tag{S68}$$

Therefore, the duality transformation connects two Ising models as

$$\sum_{j=1}^{L} \sigma_j^x \sigma_{j+1}^x + \mu\sigma_j^z = \sum_{j=1}^{L} \mathbb{Z}_j^{(2)} + \mu\mathbb{X}_j^{(2)}\mathbb{X}_{j+1}^{(2)}. \tag{S69}$$

The spin correlation function with dual y-directional spin operators between sites i and $j = i + r$ equals to the string correlation function:

$$C_{\nu=2}(r) = \left\langle \mathbb{Y}_i^{(2)}\mathbb{Y}_j^{(2)} \right\rangle_{\mathcal{G}} = \left\langle \prod_{l=i}^{j-1} \sigma_l^x \sigma_{l+1}^z \sigma_{l+2}^x \right\rangle_{\mathcal{G}}. \tag{S70}$$

Similarly, the duality transformation for topological phases with $\nu = -2$ can be written as

$$\mathbb{Z}_j^{(-2)} = \sigma_j^y \sigma_{j+1}^y, \qquad \mathbb{Y}_j^{(-2)} = \prod_{l=1}^{j} \sigma_k^z, \tag{S71}$$

$$\mathbb{X}_j^{(-2)} = -i\mathbb{Y}_j^{(-2)}\mathbb{Z}_j^{(-2)} = -\left(\prod_{l=1}^{j-1} \sigma_l^z\right) \sigma_j^x \sigma_{j+1}^y \tag{S72}$$

which implies that

$$\mathbb{X}_j^{(-2)}\mathbb{X}_{j+1}^{(-2)} = \sigma_{j+1}^z, \tag{S73}$$

and

$$\sum_{j=1}^{L} \sigma_j^y \sigma_{j+1}^y + \mu\sigma_j^z = \sum_{j=1}^{L} \mathbb{Z}_j^{(-2)} + \mu\mathbb{Y}_j^{(-2)}\mathbb{Y}_{j+1}^{(-2)}. \tag{S74}$$

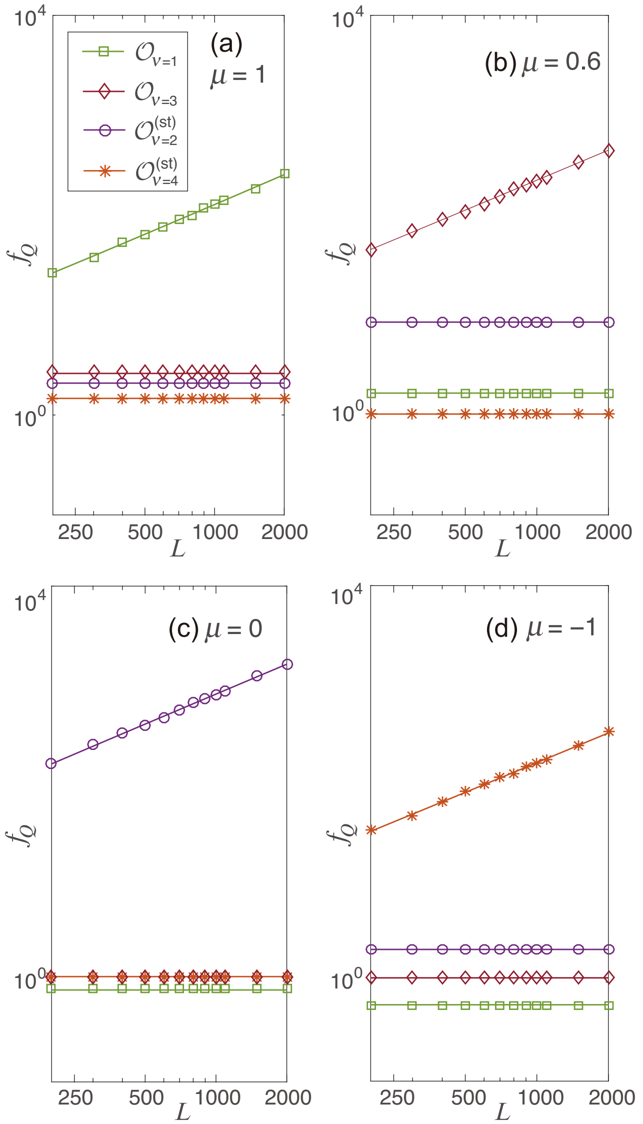

FIG. S3. (color online) Dual quantum Fisher information density f_Q of the ground state $|\mathcal{G}\rangle$ with respect to the dual generators $\mathcal{O}_\nu$ and $\mathcal{O}_\nu^{(\mathrm{st})}$ as a function of L for the extended Kitaev fermion chain with longer-range interactions and with nonzero parameters: $J_1^+ = J_1^- = 0.1$, $J_2^+ = J_2^- = 0.21$, $J_3^+ = J_3^- = -0.74$, $J_4^+ = J_4^- = 0.9$ ($N_f = 4$), in different topological phases. (a) For $\mu = 1$, the winding number $\nu = 1$, and the fitting nontrivial scaling topological index $\lambda_{\nu=1} = 0.9837$. (b) For $\mu = 0.6$, $\nu = 3$, and $\lambda_{\nu=3} = 0.9941$. (c) For $\mu = 0$, $\nu = 2$, and $\lambda^{(\mathrm{st})}_{\nu=2} = 1.0051$. (d) For $\mu = 4$, $\nu = 4$, and $\lambda^{(\mathrm{st})}_{\nu=4} = 0.9933$.

The dual x-directional correlation function between sites i and $j = i + r$ equals to the string correlation function

$$C_{\nu=-2}(r) = \left\langle \mathbb{X}_i^{(-2)} \mathbb{X}_j^{(-2)} \right\rangle_{\mathcal{G}} = \left\langle \prod_{l=i}^{j-1} \sigma_l^y \sigma_{l+1}^z \sigma_{l+2}^y \right\rangle_{\mathcal{G}}. \tag{S75}$$

We can therefore define the dual spin operators as

$$\begin{cases} \tau_j^{(2)} = \mathbb{Y}_j^{(2)}, & \text{for } \nu = 2, \\ \tau_j^{(-2)} = \mathbb{X}_j^{(-2)}, & \text{for } \nu = -2. \end{cases} \tag{S76}$$

The duality transformation for $\nu = 3$ can be written as

$$\mathbb{Z}_j^{(3)} = \sigma_j^x \sigma_{j+1}^z \sigma_{j+2}^x, \qquad \mathbb{X}_j^{(3)} = \sigma_{j+1}^x, \tag{S77}$$

$$\mathbb{Y}_j^{(3)} = -i \mathbb{Z}_j^{(3)} \mathbb{X}_j^{(3)} = \sigma_j^x \sigma_{j+1}^y \sigma_{j+2}^x \tag{S78}$$

which implies that

$$\mathbb{X}_j^{(3)} \mathbb{Z}_{j+1}^{(3)} \mathbb{X}_{j+2}^{(3)} = \sigma_{j+2}^z. \tag{S79}$$

The duality transformation for $\nu = -3$ can be written as

$$\mathbb{Z}_j^{(-3)} = \sigma_j^y \sigma_{j+1}^z \sigma_{j+2}^y, \qquad \mathbb{Y}_j^{(-3)} = \sigma_{j+1}^y, \tag{S80}$$

$$\mathbb{X}_j^{(-3)} = -i \mathbb{Y}_j^{(-3)} \mathbb{Z}_j^{(-3)} = \sigma_j^y \sigma_{j+1}^x \sigma_{j+2}^y \tag{S81}$$

which implies that

$$\mathbb{Y}_j^{(-3)} \mathbb{Z}_{j+1}^{(-3)} \mathbb{Y}_{j+2}^{(-3)} = \sigma_{j+2}^z. \tag{S82}$$

Thus, we can define the dual spin operators as

$$\begin{cases} \tau_j^{(3)} = \mathbb{Y}_j^{(3)}, & \text{for } \nu = 3, \\ \tau_j^{(-3)} = \mathbb{X}_j^{(-3)}, & \text{for } \nu = -3. \end{cases} \tag{S83}$$

Generally, the formalism of string correlation functions and dual spin operators depend on the parity of the winding numbers [25]. We first consider the odd winding numbers with $p > 1$: For positive odd winding numbers $\nu = 2p - 1$, we have

$$\mathbb{Z}_j^{(2p-1)} = \sigma_j^x \left(\prod_{l=1}^{2p-3} \sigma_{j+l}^z \right) \sigma_{j+2p-2}^x, \tag{S84}$$

$$\mathbb{X}_j^{(2p-1)} = \left(\prod_{l=1}^{p-2} \sigma_{j+2l-1}^x \sigma_{j+2l}^y \right) \sigma_{j+2p-3}^x, \tag{S85}$$

$$\mathbb{Y}_j^{(2p-1)} = \sigma_j^x \left(\prod_{l=1}^{p-1} \sigma_{j+2l-1}^y \sigma_{j+2l}^x \right), \tag{S86}$$

which implies

$$\mathbb{X}_j^{(2p-1)} \left(\prod_{l=1}^{2p-3} \mathbb{Z}_{j+l}^{(2p-1)} \right) \mathbb{X}_{j+2p-2}^{(2p-1)} = \sigma_{j+2p-2}^z. \tag{S87}$$

For negative odd winding numbers $\nu = 1 - 2p$, we have

$$\mathbb{Z}_j^{(1-2p)} = \sigma_j^y \left(\prod_{l=1}^{2p-3} \sigma_{j+l}^z \right) \sigma_{j+2p-2}^y, \tag{S88}$$

$$\mathbb{Y}_j^{(1-2p)} = \left(\prod_{l=1}^{p-2} \sigma_{j+2l-1}^y \sigma_{j+2l}^x \right) \sigma_{j+2p-3}^y, \tag{S89}$$

$$\mathbb{X}_j^{(1-2p)} = \sigma_j^y \left(\prod_{l=1}^{p-1} \sigma_{j+2l-1}^x \sigma_{j+2l}^y \right), \tag{S90}$$

which implies

$$\mathbb{Y}_j^{(1-2p)}\left(\prod_{l=1}^{2p-3}\mathbb{Z}_{j+l}^{(1-2p)}\right)\mathbb{Y}_{j+2p-2}^{(1-2p)}=\sigma_{j+2p-2}^z. \tag{S91}$$

Thus, we can define the dual spin operators as

$$\begin{cases}\tau_j^{(2p-1)}=\mathbb{Y}_j^{(2p-1)}, & \text{for } \nu=2p-1,\\ \tau_j^{(1-2p)}=\mathbb{X}_j^{(1-2p)}, & \text{for } \nu=1-2p.\end{cases} \tag{S92}$$

We then consider the even winding numbers with $p>1$: For positive even winding numbers $\nu=2p$, we have

$$\mathbb{Z}_j^{(2p)}=\sigma_j^x\left(\prod_{l=1}^{2p-2}\sigma_{j+l}^z\right)\sigma_{j+2p-1}^x, \tag{S93}$$

$$\mathbb{X}_j^{(2p)}=\left(\prod_{k=1}^{j}\sigma_k^z\right)\left(\prod_{l=1}^{p-1}\sigma_{j+2l-1}^y\sigma_{j+2l}^x\right) \tag{S94}$$

$$\mathbb{Y}_j^{(2p)}=-\left(\prod_{k=1}^{j-1}\sigma_k^z\right)\left(\prod_{l=1}^{p}\sigma_{j+2l-2}^y\sigma_{j+2l-1}^x\right) \tag{S95}$$

which implies

$$\mathbb{X}_j^{(2p)}\left(\prod_{l=1}^{2p-2}\mathbb{Z}_{j+l}^{(2p)}\right)\mathbb{X}_{j+2p-1}^{(2p)}=\sigma_{j+2p-1}^z. \tag{S96}$$

For negative even winding numbers $\nu=-2p$, we have

$$\mathbb{Z}_j^{(-2p)}=\sigma_j^y\left(\prod_{l=1}^{2p-2}\sigma_{j+l}^z\right)\sigma_{j+2p-1}^y, \tag{S97}$$

$$\mathbb{Y}_j^{(-2p)}=\left(\prod_{k=1}^{j}\sigma_k^z\right)\left(\prod_{l=1}^{p-1}\sigma_{j+2l-1}^x\sigma_{j+2l}^y\right) \tag{S98}$$

$$\mathbb{X}_j^{(-2p)}=-\left(\prod_{k=1}^{j-1}\sigma_k^z\right)\left(\prod_{l=1}^{p}\sigma_{j+2l-2}^x\sigma_{j+2l-1}^y\right) \tag{S99}$$

which implies

$$\mathbb{Y}_j^{(-2p)}\left(\prod_{l=1}^{2p-2}\mathbb{Z}_{j+l}^{(-2p)}\right)\mathbb{Y}_{j+2p-1}^{(-2p)}=\sigma_{j+2p-1}^z. \tag{S100}$$

Thus, we can write the dual spin operators as

$$\begin{cases}\tau_j^{(2p)}=\mathbb{Y}_j^{(2p)}, & \text{for } \nu=2p,\\ \tau_j^{(-2p)}=\mathbb{X}_j^{(-2p)}, & \text{for } \nu=-2p.\end{cases} \tag{S101}$$

VI. QUANTUM FISHER INFORMATION DENSITY AND STRING CORRELATION FUNCTIONS

For higher winding numbers $\nu=\pm2,\pm3,\cdots$, the quantum Fisher information with respect to the dual generators

$$\mathcal{O}_\nu=\sum_{j=1}^{M}\tau_j^{(\nu)},\qquad \mathcal{O}_\nu^{(\mathrm{st})}=\sum_{j=1}^{M}(-)^j\tau_j^{(\nu)} \tag{S102}$$

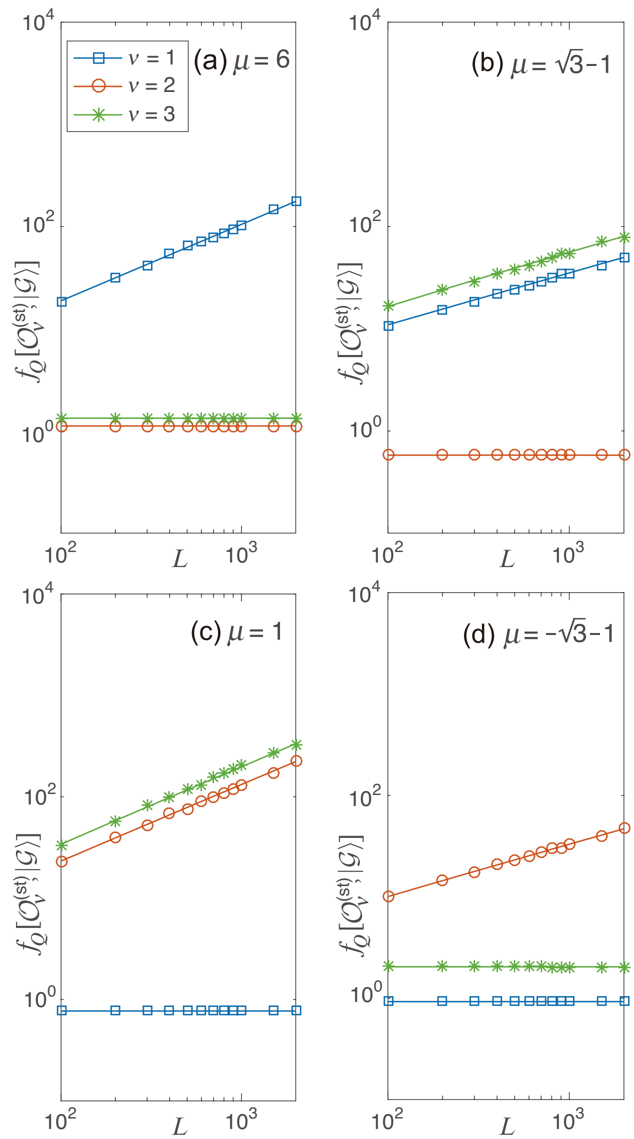

FIG. S4. (color online) Quantum Fisher information density $f_Q[\mathcal{O}_\nu^{(\mathrm{st})},|\mathcal{G}\rangle]$ as a function of L for the extended Kitaev fermion chain with nonzero parameters $J_1^+=J_1^-=1$, $J_2^+=J_2^-=2$, $J_3^+=J_3^-=2$ ($N_f=3$) on the contour between different topological phases for (a) $\mu=5$, (b) $\mu=\sqrt{3}-1$, (c) $\mu=-1$, and (d) $\mu=-\sqrt{3}-1$. The scaling coefficients $\lambda_\nu^{(\mathrm{st})}$ are shown in Tab. II.

can be written as

$$F_Q[\mathcal{O}_\nu,|\mathcal{G}\rangle]=M+M\sum_{r=1}^{M-1}\langle\tau_i^{(\nu)}\tau_{i+r}^{(\nu)}\rangle_{\mathcal{G}} \tag{S103}$$

$$F_Q[\mathcal{O}_\nu^{(\mathrm{st})},|\mathcal{G}\rangle]=M+M\sum_{r=1}^{M-1}(-)^r\langle\tau_i^{(\nu)}\tau_{i+r}^{(\nu)}\rangle_{\mathcal{G}} \tag{S104}$$

where $(\tau_j^{(\nu)})^2=\mathbb{I}$, with $\mathbb{I}$ the identity, and we let

$$M\equiv L-|\nu|+1. \tag{S105}$$

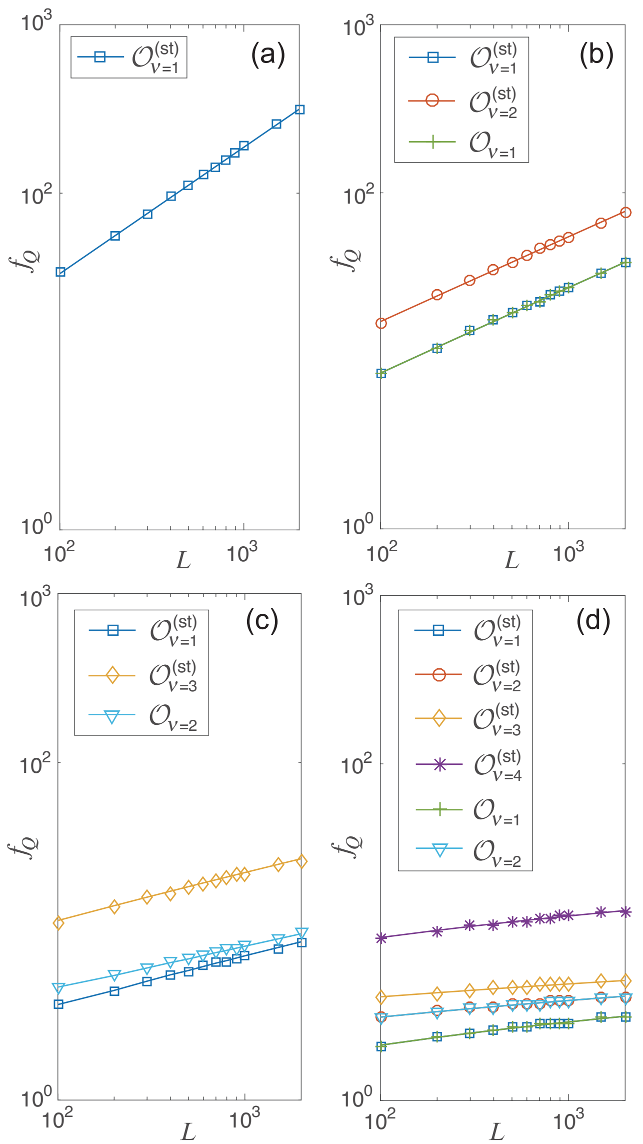

FIG. S5. (color online) Quantum Fisher information density f_Q of the ground state $|\mathcal{G}\rangle$ with respect to the dual generators $\mathcal{O}_\nu$ and $\mathcal{O}_\nu^{(\mathrm{st})}$ as a function of L for the extended Kitaev fermion chain when $\mu = 1$ with nonzero parameters: (a) $J_1^+ = J_1^- = 1$ ($N_f = 1$); (b) $J_2^+ = J_2^- = 1$ ($N_f = 2$); (c) $J_3^+ = J_3^- = 1$ ($N_f = 3$); and (d) $J_4^+ = J_4^- = 1$ ($N_f = 4$). The scaling coefficients λ_ν and $\lambda_\nu^{(\mathrm{st})}$ are shown in Tab. III.

For the thermodynamic limit $L \gg N_f \geq 1$, we can obtain the dual quantum Fisher information density as

$$f_Q[\mathcal{O}_\nu, |\mathcal{G}\rangle] = \frac{F_Q[\mathcal{O}_\nu, |\mathcal{G}\rangle]}{L} = 1 + \sum_{r=1}^{L-|\nu|} C_\nu(r), \tag{S106}$$

$$f_Q[\mathcal{O}_\nu^{(\mathrm{st})}, |\mathcal{G}\rangle] = \frac{F_Q[\mathcal{O}_\nu^{(\mathrm{st})}, |\mathcal{G}\rangle]}{L} = 1 + \sum_{r=1}^{L-|\nu|} (-)^r C_\nu(r), \tag{S107}$$

where $M \simeq L$ as $|\nu| \leq N_f$, and

$$C_\nu(r) \equiv \langle \tau_i^{(\nu)} \tau_{i+r}^{(\nu)} \rangle_{\mathcal{G}} \tag{S108}$$

is the so-called string correlation function [22, 23] from site i to $j = i + r$ in the dual lattice. The string correlation function is shown able to reveal hidden symmetry-protected order by $\mathbf{Z}$ symmetry in many topological systems [19, 20, 22, 23]. It is easier to rewrite the string correlation function in terms of Majorana operators and fermion operators

$$d_{l,\nu} = (b_l + i a_{l+\nu})/2, \qquad d_{l,\nu}^\dagger = (b_l - i a_{l+\nu})/2 \tag{S109}$$

as

$$C_\nu(r) = \left\langle \prod_{l=i}^{j-1} (-i b_l a_{l+\nu}) \right\rangle_{\mathcal{G}} = \left\langle \prod_{l=i}^{j-1} (1 - 2 d_{l,\nu}^\dagger d_{l,\nu}) \right\rangle_{\mathcal{G}}. \tag{S110}$$

Usually, the string correlation function is written in terms of Pauli matrices as

$$C_\nu(r) = \left\langle \prod_{l=i}^{j-1} \left(\sigma_l^\alpha \sigma_{l+|\nu|}^\alpha \prod_{k=l+1}^{l+|\nu|-1} \sigma_k^z \right) \right\rangle_{\mathcal{G}}, \tag{S111}$$

where $\alpha = x$ for positive ν, and $\alpha = y$ for negative ν.

The interchange between the quantum phases with positive and negative winding numbers $\nu = \pm n$ (n is a positive integer)

$$\mathcal{O}_{\nu=n}^{(\mathrm{st})} \leftrightarrow \mathcal{O}_{\nu=-n}^{(\mathrm{st})}, \qquad \mathcal{O}_{\nu=n} \leftrightarrow \mathcal{O}_{\nu=-n} \tag{S112}$$

$$f_Q[\mathcal{O}_{\nu=n}^{(\mathrm{st})}] \leftrightarrow f_Q[\mathcal{O}_{\nu=-n}^{(\mathrm{st})}], \qquad f_Q[\mathcal{O}_{\nu=n}] \leftrightarrow f_Q[\mathcal{O}_{\nu=-n}] \tag{S113}$$

can be realized by a phase redefinition $c_j \to \pm i c_j$.

Another interchange between the staggered operator $\mathcal{O}_{\nu=1}^{(\mathrm{st})}$ and the operator $\mathcal{O}_{\nu=1}$, for the positive and negative signs of the interaction between Dirac fermions localized at the chain ends, respectively,

$$\mathcal{O}_{\nu=n}^{(\mathrm{st})} \leftrightarrow \mathcal{O}_{\nu=n}, \qquad \mathcal{O}_{\nu=-n}^{(\mathrm{st})} \leftrightarrow \mathcal{O}_{\nu=-n} \tag{S114}$$

$$f_Q[\mathcal{O}_{\nu=n}^{(\mathrm{st})}] \leftrightarrow f_Q[\mathcal{O}_{\nu=n}], \qquad f_Q[\mathcal{O}_{\nu=-n}^{(\mathrm{st})}] \leftrightarrow f_Q[\mathcal{O}_{\nu=-n}] \tag{S115}$$

can be realized by a Hermitian conjugate transformation $c_j \to c_j^\dagger$.

Following the calculations in previous sections, we can write the string correlation function into a determinant of size $(r - |\nu| + 1)$ as

$$C_\nu(r) = \begin{vmatrix} G_{-\nu} & G_{-\nu-1} & \cdots & G_{-r} \\ G_{1-\nu} & G_{-\nu} & \cdots & G_{1-r} \\ \vdots & \vdots & \vdots & \vdots \\ G_{r-2\nu} & G_{r-2\nu+1} & \cdots & G_{-\nu} \end{vmatrix} \tag{S116}$$

for positive ν and

$$C_\nu(r) = \begin{vmatrix} G_{-\nu} & G_{-\nu-1} & \cdots & G_{-r-2\nu} \\ G_{1-\nu} & G_{-\nu} & \cdots & G_{1-r-2\nu} \\ \vdots & \vdots & \vdots & \vdots \\ G_{r} & G_{r-1} & \cdots & G_{-\nu} \end{vmatrix} \tag{S117}$$

for negative ν.

Because the string correlation function decays exponentially versus the distance r when breaking the hidden $\mathbf{Z}$ symmetry (see, for example, Fig. S2), the quantum Fisher information density as a function of L has a scaling form in the thermodynamic limit,

$$f_Q[\mathcal{O}_\nu, |\mathcal{G}\rangle] \simeq 1 + \gamma_\nu L^{\lambda_\nu}, \tag{S118}$$

$$f_Q[\mathcal{O}_\nu^{(\mathrm{st})}, |\mathcal{G}\rangle] \simeq 1 + \gamma_\nu^{(\mathrm{st})} L^{\lambda_\nu^{(\mathrm{st})}} \tag{S119}$$

and becomes linear:

$$\lambda_\nu \text{ or } \lambda_\nu^{(\mathrm{st})} \simeq 1 \tag{S120}$$

in the topological quantum phase with a winding number ν and constant:

$$\lambda_\nu \text{ and } \lambda_\nu^{(\mathrm{st})} \simeq 0, \tag{S121}$$

in the other phases, see Fig. S3 for example. Thus, the scaling coefficient λ_ν or $\lambda_\nu^{(\mathrm{st})}$ obtained by numerical calculations can identify the topological phases with higher winding numbers, see numerical results in Tab. I.

VII. TOPOLOGICAL PHASE TRANSITIONS AND HALF-INTEGER WINDING NUMBERS WITH ZEROS ON THE CRITICAL CONTOUR

For completeness, we discuss the case when zeros of the characteristic equation appear on the contour $|\zeta| = 1$, and interpret the physical implications of half-integer winding numbers therein. We can find that the topological phase transitions occur at the critical points satisfying

$$g(\zeta) = \sum_{n=1}^{N_f} (J_n^x \zeta^n + J_n^y \zeta^{-n}) - \mu = 0 \tag{S122}$$

μ	$\lambda_{\nu=1}^{(\mathrm{st})}$	$\lambda_{\nu=2}^{(\mathrm{st})}$	$\lambda_{\nu=3}^{(\mathrm{st})}$
6[a]	2.8×10^{-5}	-4.3×10^{-7}	-1.6×10^{-6}
3	0.9965	9.4×10^{-14}	2.5×10^{-13}
0	-4.2×10^{-14}	1.4×10^{-13}	1.0047
-2	-5.6×10^{-7}	0.9957	2.9×10^{-7}
5[b]	0.7492	4.1×10^{-7}	-1.9×10^{-6}
$\sqrt{3} - 1$	0.5054	-2.8×10^{-3}	0.5165
-1	6.8×10^{-5}	0.7518	0.7547
$-\sqrt{3} - 1$	1.0×10^{-3}	0.5088	-5.6×10^{-4}

[a] Inside topological phases.
[b] On the critical contour between phases.

TABLE II. Fitting of the scaling coefficients $\lambda_\nu^{(\mathrm{st})}$ of the dual quantum Fisher information density $f_Q[\mathcal{O}_\nu^{(\mathrm{st})}, |\mathcal{G}\rangle]$ inside different topological phases and on the critical contour between phases for the extended Kitaev fermion chain with nonzero parameters $J_1^+ = J_1^- = 1$, $J_2^+ = J_2^- = 2$, $J_3^+ = J_3^- = 2$ ($N_f = 3$), and chain length up to $L = 2000$. The nine essentially non-zero scaling coefficients are show in blue font.

for $|\zeta| = 1$.

For example, we choose the parameters of the extended Kitaev fermion chain as $J_1^+ = J_1^- = 1$, $J_2^+ = J_2^- = 2$, $J_3^+ = J_3^- = 2$ ($N_f = 3$), and calculate the real solutions of the chemical potential μ: for $\zeta = 1$, $\mu = 5$; for $\zeta = -1$, $\mu = -1$; for

$$\zeta = \exp\{\pm i \arccos[(-\sqrt{3} - 1)/4]\}, \tag{S123}$$

$\mu = \sqrt{3} - 1$; and for

$$\zeta = \exp\{\pm i \arccos[(\sqrt{3} - 1)/4]\}, \tag{S124}$$

$\mu = -\sqrt{3} - 1$, where the topological phase transitions occur. For another example, we consider the parameters of the extended Kitaev fermion chain as $J_2^+ = J_2^- = \lambda$, $J_1^+ = 1$, $J_1^- = -1$, $\mu = 1$, and change the value of λ. We can obtain the critical points of topological phase transitions by solving the characteristic equation:

$$g(\zeta) = \lambda \zeta^2 + \zeta^{-1} - 1 = 0 \tag{S125}$$

where we can obtain the transition points: for $\zeta = 1$, $\lambda = 0$; for $\zeta = -1$, $\lambda = 2$; for

$$\zeta = \exp\{\pm i \arccos[(1 - \sqrt{5})/4]\}, \tag{S126}$$

$\lambda = (-\sqrt{5} - 1)/2$; and for

$$\zeta = \exp\{\pm i \arccos[(1 + \sqrt{5})/4]\}, \tag{S127}$$

$\lambda = (\sqrt{5} - 1)/2$.

We then consider the critical behaviors of quantum states on the transition points. From the viewpoint of geometric topology, we consider the Kitaev closed chain as $\Delta = J$ and assume an anti-periodic boundary conditions $c_{j+L} = -c_j$. If

$$\Delta = -\mu = -1, \tag{S128}$$

the characteristic function becomes

$$g(\zeta) = \zeta - 1, \tag{S129}$$

and the winding number can be calculated by the Cauchy principal value:

$$\nu = \frac{1}{2\pi i} \oint_{|\zeta|=1} d\zeta \, \frac{1}{\zeta - 1} \tag{S130}$$

$$= \frac{1}{2\pi i} \lim_{\varepsilon \to 0} \left[\int_{-\varepsilon}^{2\pi - \varepsilon} d\zeta \, \frac{1}{\zeta - 1} \right]$$

$$= \frac{1}{2\pi i} \lim_{\varepsilon \to 0} \left[i\varepsilon \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} d\theta \, \frac{e^{i\theta}}{(\varepsilon e^{i\theta} + 1) - 1} \right] \tag{S131}$$

$$= \frac{1}{2}, \tag{S132}$$

where we can only obtain massive Dirac edge modes [26] for the open Kitaev chain. Moreover, in consideration of the boundary parts for the closed chain, we can write the Hamiltonian in terms of Majorana fermion operators as

$$iH = \sum_{j=1}^{L} a_j b_j + \sum_{j=1}^{L-1} b_j a_{j+1} + (-1)^{N_p} b_L a_1, \tag{S133}$$

$g(\zeta)$	$\lambda^{(\mathrm{st})}_{\nu=1}$	$\lambda_{\nu=1}$	$\lambda^{(\mathrm{st})}_{\nu=2}$	$\lambda_{\nu=2}$	$\lambda^{(\mathrm{st})}_{\nu=3}$	$\lambda_{\nu=3}$	$\lambda^{(\mathrm{st})}_{\nu=4}$	$\lambda_{\nu=4}$
$\zeta-1$	0.7506	$<10^{-5}$	$<10^{-5}$	$<10^{-3}$	$<10^{-5}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$
ζ^2-1	0.5072	0.5072	0.5040	$<10^{-4}$	$<10^{-3}$	$<10^{-16}$	$<10^{-4}$	$<10^{-16}$
ζ^3-1	0.2873	0.0043	$<10^{-3}$	0.2441	0.2809	$<10^{-16}$	$<10^{-3}$	$<10^{-16}$
ζ^4-1	0.1313	0.1313	0.0950	0.0950	0.0745	$<10^{-16}$	0.1223	$<10^{-16}$

TABLE III. Fitting of the scaling coefficients λ_ν and $\lambda_\nu^{(\mathrm{st})}$ with respect to the dual generators $\mathcal{O}_\nu$ and $\mathcal{O}_\nu^{(\mathrm{st})}$, respectively, on the critical contour between phases for the extended Kitaev fermion chain with characteristic functions $g(\zeta)$ and chain length up to $L=2000$. The thirteen essentially non-zero scaling coefficients are shown in blue font.

where we have that

$$\phi=\frac{1}{\sqrt{L}}\sum_{j=1}^{L}a_j,\qquad \psi=\frac{1}{\sqrt{L}}\sum_{j=1}^{L}b_j, \tag{S134}$$

are a pair of zero modes (obviously not edge modes) for even N_p, but there exists no zero mode for odd parity. Therefore, the half-integer winding number represents a critical phenomenon when the Majorana zero mode exists or not for different fermion parities $(-1)^{N_p}$ in consideration of boundary Hamiltonian. Generally, it can be inferred that if we have even number of zeros on the contour, the winding number is still an integer for different fermion parities.

In Fig. S4, we plot the quantum Fisher information density as a function of L in critical cases for the extended Kitaev fermion chain with $J_1^+=J_1^-=1$, $J_2^+=J_2^-=2$, $J_3^+=J_3^-=2$ ($N_f=3$), and present the scaling coefficients $\lambda_\nu^{(\mathrm{st})}$ in Tab. II. Then, we plot in Fig. S5 the quantum Fisher information density as a function of L for an extended Kitaev fermion chain with characteristic functions:

(a) $g(\zeta)=\zeta-1$,

(b) $g(\zeta)=\zeta^2-1$,

(c) $g(\zeta)=\zeta^3-1$,

(d) $g(\zeta)=\zeta^4-1$,

where the zeros are on the contour $|\zeta|=1$ given $\mu=1$. The scaling coefficients λ_ν and $\lambda_\nu^{(\mathrm{st})}$ are shown in Tab. III. We should note that our discussions would be inappropriate to discuss the Dirac sector of the topological phase diagram for the extended Kitaev chain which would have a half integer winding number [11, 26–28], because the boundary conditions (anti-periodic and periodic) for finite chain length L would destroy long-range hopping and pairing terms, and the thermodynamic limit $L\gg N_f\geq 1$ could not be satisfied.

VIII. CHARACTERIZATION OF TOPOLOGICAL PHASES IN A KITAEV HONEYCOMB MODEL VIA DUAL MULTIPARTITE ENTANGLEMENT

The Kitaev honeycomb model (i.e., a two-dimensional spin model on a hexagonal lattice with direction-dependent interactions between adjacent lattice sites) is an analytically solvable model with topological quantum phase transitions at zero temperature [29]. The Hamiltonian is

$$H_{\mathrm{hc}}=-\sum_{\kappa=x,y,z}J_\kappa\sum_{\langle ij\rangle_\kappa}\sigma_i^\kappa\sigma_j^\kappa, \tag{S135}$$

where $\langle ij\rangle_\kappa$ denotes the nearest-neighbor bonds in the κ-direction. At each site, we define four Majorana operators a^α, with $\alpha=0,x,y,z$, satisfying $(a^\alpha)^\dagger=a^\alpha$, $\{a^\alpha,a^\beta\}=2\delta_{\alpha\beta}$, and $a^xa^ya^za^0=1$, and write the Pauli operators as

$$\sigma_j^\kappa=ia_j^\kappa a_j, \tag{S136}$$

with $\kappa=x,y,z$ and $a_j^0\equiv a_j$. The Hamiltonian is then rewritten with

$$\hat{u}_{\langle ij\rangle_\kappa}\equiv ia_i^\kappa a_j^\kappa \tag{S137}$$

as

$$H_{\mathrm{hc}}=\frac{i}{2}\sum_{\langle ij\rangle_\kappa}J_{\kappa_{\langle ij\rangle}}\hat{u}_{\langle ij\rangle_\kappa}a_ia_j, \tag{S138}$$

where the factor $\frac{1}{2}$ is due to each lattice being counted twice in the summation. We have $\hat{u}^2_{\langle ij\rangle_\kappa}=1$ and $[H_{\mathrm{hc}},\hat{u}_{\langle ij\rangle_\kappa}]=0$. Here we take $\hat{u}_{\langle ij\rangle_\kappa}=1$ for all bonds (π-flux phase), because this vortex-free configuration has the lowest energy [29, 30]. The system size is $N=2LM$, and at first, we set $M=L$.

Using the Fourier transformation, the Hamiltonian in the momentum representation is [31]

$$H_{\mathrm{hc}}=\sum_{\boldsymbol{q}}(a_{-\boldsymbol{q},1},a_{-\boldsymbol{q},2})\,\mathcal{H}_{\boldsymbol{q}}\begin{pmatrix}a_{\boldsymbol{q},1}\\ a_{\boldsymbol{q},2}\end{pmatrix}, \tag{S139}$$

where $\boldsymbol{q}=(q_1,q_2)$ is the momentum vector and the Bloch matrix of $\mathcal{H}_{\boldsymbol{q}}$ is

$$\mathcal{H}_{\boldsymbol{q}}=-\Delta_{\boldsymbol{q}}\sigma^x-\epsilon_{\boldsymbol{q}}\sigma^y=\begin{pmatrix}0 & i\Upsilon_{\boldsymbol{q}}\\ -i\Upsilon^*_{\boldsymbol{q}} & 0\end{pmatrix}, \tag{S140}$$

with

$$\Upsilon_{\boldsymbol{q}}=\epsilon_{\boldsymbol{q}}+i\Delta_{\boldsymbol{q}}, \tag{S141}$$
$$\epsilon_{\boldsymbol{q}}=J_x\cos q_1+J_y\cos q_2+J_z, \tag{S142}$$
$$\Delta_{\boldsymbol{q}}=J_x\sin q_1+J_y\sin q_2. \tag{S143}$$

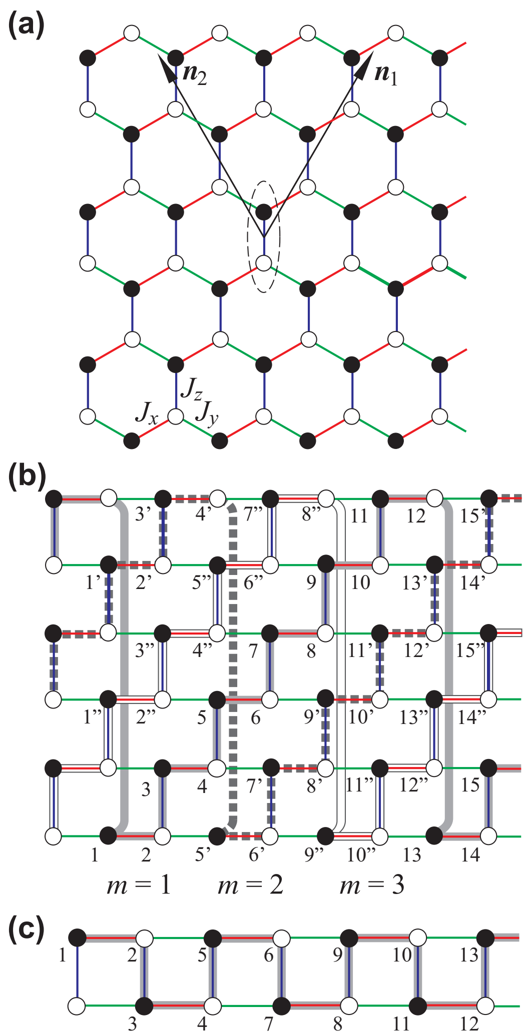

FIG. S6. (color online) (a) A graphic representation of the Kitaev honeycomb model with two sublattices (empty and full circles). There are three types of bonds labeled by x, y, z. (b) The equivalent brick-wall lattice with three rows ($m = 1, 2, 3$). (c) A single-chain representation of the two-leg spin ladder.

By choosing the coordinate axes in the $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$ directions as shown in Fig. S6(a), then the momentum vectors $q_1 = \boldsymbol{q}\cdot\boldsymbol{n}_1$ and $q_2 = \boldsymbol{q}\cdot\boldsymbol{n}_2$ take the values

$$q_{1,2} = \frac{2l\pi}{L}, \qquad l = -\frac{L-1}{2}, \cdots, \frac{L-1}{2}. \tag{S144}$$

Using the Bogoliubov transformation

$$D_{\boldsymbol{q},1} = u_{\boldsymbol{q}} a_{\boldsymbol{q},1} + v_{\boldsymbol{q}} a_{\boldsymbol{q},2}, \qquad D_{\boldsymbol{q},2} = v^*_{\boldsymbol{q}} a_{\boldsymbol{q},1} - u^*_{\boldsymbol{q}} a_{\boldsymbol{q},2} \tag{S145}$$

with $u_{\boldsymbol{q}} = 1/\sqrt{2}$ and $v_{\boldsymbol{q}} = i\Upsilon_{\boldsymbol{q}}/(\sqrt{2}|\Upsilon_{\boldsymbol{q}}|)$, the Hamiltonian is diagonalized

$$H_{\rm hc} = \sum_{\boldsymbol{q}} |f_{\boldsymbol{q}}|(1 - 2D^\dagger_{\boldsymbol{q},2} D_{\boldsymbol{q},2}), \tag{S146}$$

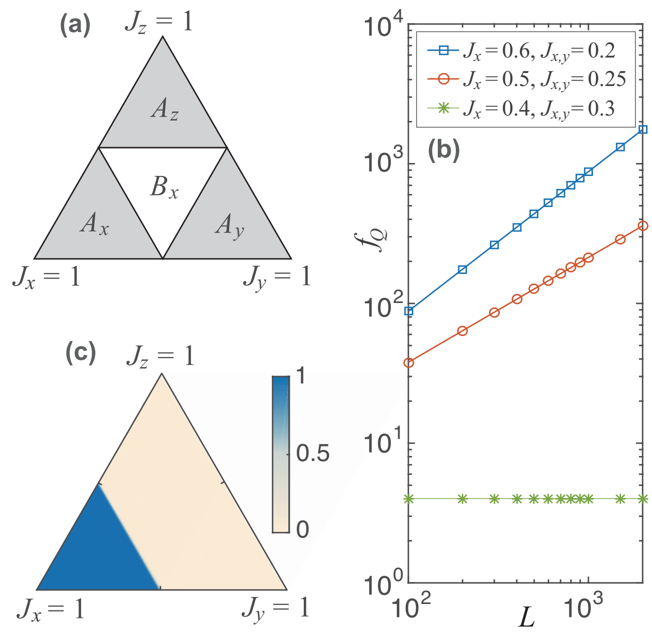

FIG. S7. (color online) (a) The phase diagram of the Kitaev honeycomb model in the $J_x + J_y + J_z = 1$ plane. (b) Quantum Fisher information density in the dual lattice as a function of L for the two-leg spin ladder. The scaling coefficients are $\lambda_x^{(\rm st)} \simeq 0.9992$ for $J_{x,y,z} = 0.6, 0.2, 0.2$, $\lambda_x^{(\rm st)} \simeq 0.7508$ for $J_{x,y,z} = 0.5, 0.25, 0.25$, and $\lambda_x^{(\rm st)} < 10^{-12}$ for $J_{x,y,z} = 0.4, 0.3, 0.3$. (c) Scaling topological index $\lambda_x^{(\rm st)}$ with different values of $J_{x,y,z}$ in the $J_x + J_y + J_z = 1$ plane versus the system size $2L$ up to 400.

where we have used $\{D^\dagger_{\boldsymbol{q},\mu}, D^\dagger_{\boldsymbol{q}',\mu'}\} = \delta_{\boldsymbol{q},\boldsymbol{q}'}\delta_{\mu,\mu'}$, $D^2_{\boldsymbol{q},\mu} = 0$, and $D^\dagger_{\boldsymbol{q},1} D_{\boldsymbol{q},1} = 1 - D^\dagger_{\boldsymbol{q},2} D_{\boldsymbol{q},2}$. The ground state is

$$|\mathcal{G}\rangle = \prod_{\boldsymbol{q}} D^\dagger_{\boldsymbol{q},2}|0\rangle \tag{S147}$$

and the energy gap is $2\min_{\boldsymbol{q}}\{|\Upsilon_{\boldsymbol{q}}|\}$.

Then, we consider positive bonds, $J_{x,y,z} > 0$, and focus on the $J_x + J_y + J_z = 1$ parametric plane. As presented in Fig. S7(a), in the region of $J_x \le J_y + J_z$, $J_y \le J_z + J_x$ and $J_z \le J_x + J_y$, there is a gapless phase B with non-Abelian excitations, and in other regions, there are three gapped phases with Abelian anyon excitations [29]

$$A_x: \; J_x \ge J_y + J_z, \tag{S148}$$
$$A_y: \; J_y \ge J_z + J_x, \tag{S149}$$
$$A_z: \; J_z \ge J_x + J_y. \tag{S150}$$

Following [20], we consider a two-leg spin ladder of the Kitaev honeycomb model and relabel all the sites along a special path [as shown in Fig. S6(c)] and express the Hamiltonian with the third-nearest-neighbor couplings [20]

$$H_{2l} = -\sum_{j=1}^{L}(J_x\sigma^x_{2j-1}\sigma^x_{2j} + J_y\sigma^y_{2j}\sigma^y_{2j+3} + J_z\sigma^z_{2j}\sigma^z_{2j+1}). \tag{S151}$$

By considering the duality transformation introduced in [20]

$$\sigma_j^x = \check{s}_{j-1}^x \check{s}_j^x, \qquad \sigma_j^z = \prod_{k=j}^{2L} \check{s}_k^z, \tag{S152}$$

$$\sigma_j^y = -i\sigma_j^z \sigma_j^x = \check{s}_{j-1}^x \check{s}_j^y \prod_{k=j+1}^{2L} \check{s}_k^z, \tag{S153}$$

we obtain an anisotropic XY spin chain with a transverse field in the dual space

$$H_{2l} = -\sum_{j=1}^{L} (J_x \check{s}_{2j}^x \check{s}_{2j+2}^x + J_y W_j \check{s}_{2j}^y \check{s}_{2j+2}^y + J_z \check{s}_{2j}^z), \tag{S154}$$

where

$$W_j = \check{s}_{2j-1}^x \check{s}_{2j+1}^z \check{s}_{2j+3}^x \tag{S155}$$

is the plaquette operator in the dual lattice and a good quantum number [20]. We have $W_j = -1$ (π-flux phase [30]) for the ground state. We consider the inverse dual transformation

$$\check{s}_j^x = \prod_{k=1}^{j} \sigma_k^x, \qquad \check{s}_j^z = \sigma_j^z \sigma_{j+1}^z \tag{S156}$$

$$\check{s}_j^y = -i\check{s}_j^z \check{s}_j^x = \sigma_{j+1}^z \sigma_j^y \prod_{k=1}^{j-1} \sigma_k^x \tag{S157}$$

and consider the spin correlation function in the dual lattice

$$C_x(r) \equiv \langle \check{s}_{2i}^x \check{s}_{2j}^x \rangle_{\mathcal{G}} = \left\langle \prod_{k=2i+1}^{2j} \sigma_k^x \right\rangle_{\mathcal{G}} \tag{S158}$$

where $r = j - i$. It is shown in Ref. [20] that the string correlation order

$$\lim_{r\to\infty} (-)^r C_x(r) \neq 0 \tag{S159}$$

in the phase A_x ($J_x \geq J_y + J_z$) and equals to zero in other regions. Similarly, with respect to the dual generator

$$\mathcal{O}_x^{(\mathrm{st})} = \sum_{j=1}^{L} (-)^j \check{s}_{2j}^x, \tag{S160}$$

the quantum Fisher information density in the dual lattice is

$$f_Q[\mathcal{O}_x^{(\mathrm{st})}, |\mathcal{G}\rangle] \equiv 1 + \sum_{r=1}^{L-1} (-)^r C_x(r) \tag{S161}$$

$$\simeq 1 + \gamma_x^{(\mathrm{st})} L^{\lambda_x^{(\mathrm{st})}}. \tag{S162}$$

In the gapped phase A_x, the dual QFI density is linear

$$\lambda_x^{(\mathrm{st})} \simeq 1 \tag{S163}$$

and constant

$$\lambda_x^{(\mathrm{st})} \simeq 0 \tag{S164}$$

in other regions, see Fig. S7(b,c) for example. Moreover, the gapped phases A_y and A_z as shown in Fig. S7(a) can be obtained by the substitutions $J_x \to J_y \to J_z \to J_x$ and $J_x \to J_z \to J_y \to J_x$, respectively. Therefore, the scaling coefficient of the dual quantum Fisher information density in the dual lattice can identify three gapped phases A_x, A_y and A_z with Abelian anyon excitations.

Generally, we consider the equivalent brick-wall lattice of the Kitaev honeycomb model as shown in Fig. S6(b) and rewrite the Hamiltonian (S135) as

$$H_{\mathrm{hc}} = -\sum_{j=1}^{L} \sum_{m=1}^{M} (J_x \sigma_{2j-1,m}^x \sigma_{2j,m}^x + J_y \sigma_{2j,m}^y \sigma_{2j+3,m+1}^y + J_z \sigma_{2j,m}^z \sigma_{2j+1,m}^z). \tag{S165}$$

In the two-dimensional limit $M \to \infty$, the above results for the two-leg spin ladder using string correlation functions and dual quantum Fisher information density to detect topological phase transitions can also be extended to the general two-dimensional lattice by transforming the second index m to momentum space [20].

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