Majorana edge magnetization in the Kitaev honeycomb model

Tomonari Mizoguchi\textsuperscript{1,}\,\textsuperscript{*} and Tohru Koma\textsuperscript{2,}\,\textsuperscript{†}

\textsuperscript{1}Department of Physics, University of Tsukuba, Tsukuba, Ibaraki 305-8571, Japan
\textsuperscript{2}Department of Physics, Gakushuin University, Mejiro, Toshima-ku, Tokyo 171-8588, Japan

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We propose an approach to detect the peculiarity of Majorana fermions at the edges of Kitaev magnets. As is well known, a pair of Majorana edge modes is realized when a single complex fermion splits into real and imaginary parts which are, respectively, localized at the left and right edges of a sample magnet. Reflecting both of this peculiarity of the Majorana fermions and the ground-state degeneracy caused by the existence of the Majorana edge zero modes, the spins at the edges of the sample magnet are expected to behave as a peculiar “free” spin which exhibits a unidirectional magnetization without any transverse magnetization when applied a sufficiently weak external magnetic field. For the Kitaev honeycomb model, we obtain the expression of the Majorana edge magnetization by relying on standard techniques to diagonalize a free fermion Hamiltonian. The magnetization profile thus obtained indeed shows the expected behavior. We also elucidate the relation between the Majorana edge flat band and the bulk winding number from a weak topological point of view.

I. INTRODUCTION

Kitaev introduced a seminal quantum spin model\textsuperscript{[1]} which realizes the desired properties of quantum spin liquids\textsuperscript{[2, 3]}, whose study was initiated by Anderson. More precisely, Kitaev’s model is defined on the honeycomb lattice, and mapped to a free Majorana fermion model. In consequence, the model is exactly solvable, and shows short-range spin correlations\textsuperscript{[4]}. Although Kitaev’s model is fairly artificial, some materials, e.g., $A_2\text{IrO}_3$ ($A = \text{Na, Li}$)\textsuperscript{[5, 6]} and $\alpha$-RuCl$_3$\textsuperscript{[7]}, are expected to exhibit very similar properties to those of the Kitaev honeycomb model\textsuperscript{[8–12]}. In particular, detecting the evidence of the Majorana fermions is one of the central issues in condensed matter physics\textsuperscript{[13–19]}. On the other hand, the Kitaev honeycomb model with open boundaries shows many Majorana zero modes at the edges\textsuperscript{[20]}. In fact, the zero modes form a flat band. This is nothing but a consequence of the weak topological character\textsuperscript{[21–26]} of the model. In fact, the celebrated bulk-edge correspondence\textsuperscript{[27, 28]} ensures the relation between the number of the Majorana edge zero modes and the winding number for the bulk Hamiltonian when the Fermi energy, which equals zero in the present system, lies in the spectral or mobility gap of the Hamiltonian. Interestingly, similar Majorana edge flat bands were found to appear also in the gapless regime of the Hamiltonian, depending on the geometry of the edges\textsuperscript{[20]}. As is well known, a pair of Majorana edge modes appears when a single complex fermion splits into real and imaginary parts which are, respectively, localized at the left and right edges of the system. Therefore, a single Majorana fermion has only a real degree of freedom as an internal degree of freedom. Reflecting this peculiarity of the Majorana fermions and the ground-state degeneracy caused by the existence of the Majorana edge zero modes, the spins at the edges of the Kitaev honeycomb model are expected to behave as a peculiar “free” spin which exhibits a unidirectional magnetization without any transverse magnetization when applied a sufficiently weak external magnetic field. Thus, the edge magnetization is expected to serve as a probe to detect the signature of the Majorana edge modes.

In the present paper, we derive the expression of the edge magnetization in the bulk gapped regime of the Kitaev honeycomb model on the cylinder geometry with the open boundary condition, by using standard techniques to diagonalize a free-fermion Hamiltonian. As a result, we show that the profile of the edge magnetization indeed exhibits the desired properties. More precisely, the magnetization is perfectly unidirectional, namely, only a single component of the expectation value of the three

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{The Kitaev honeycomb model with edges in the horizontal direction. Red, blue, and green bonds represent $x$-, $y$-, and $z$-bonds, respectively. Black (white) circles denote the sites with an odd (even) $\ell$.}
\end{figure}
component spin operator can be non-vanishing, while the rest two components must be vanishing. This is nothing but a consequence of the fractionalization of a single spin into two independent Majorana fermions.

We also elucidate the relation between the Majorana edge flat band and the weak topological character of the Kitaev honeycomb model. The latter is characterized by the winding number for the Hamiltonian on the infinitely-long cylinder with a finite radius. Due to the topological character, the Majorana edge flat band can be proved to be stable against disorders which preserve the symmetry of the Hamiltonian. Further, we can expect that the Majorana edge flat band is stable against additional interactions.

The rest of this paper is organized as follows. In Sec. II, we give the precise definition of the Kitaevs honeycomb model with the cylinder geometry, which is periodic in the vertical direction and has two edges in the horizontal direction. The model is mapped to a fermion model by using the Jordan-Wigner transformation. In Sec. III, for the model with the cylinder geometry, we derive zero-energy edge states in the momentum space. Further, from these states, we construct Wannier orbitals, which are useful for calculating the local quantities. In Sec. IV, we compute the edge magnetization by explicitly calculating the expectation value of the spin operator by using the Wannier orbitals. Section V is devoted to discussions which include the stability of the Majorana edge flat band and the weak topological character of the Kitaev honeycomb model. The latter is characterized by the winding number for the Hamiltonian on the infinitely-long cylinder with a finite radius. Due to the topological condition in the horizontal direction and the periodic boundary condition in the vertical direction in Fig. 1. Namely, we consider the cylinder geometry with two zigzag edges. Clearly, one can notice that the sites, denoted by black and white circles in Fig. 1, are placed on the two-dimensional square lattice. Therefore, we can label a site \( i \) by \( i = (\ell, m) \) with two positive integers, \( \ell \) and \( m \), which satisfy \( 1 \leq \ell \leq 2L_x \) and \( 1 \leq m \leq L_y \) with the length \( 2L_x \) of the cylinder and the length \( L_y \) of the circumference of the cylinder.

The Hamiltonian of Eq. (1) can be transformed to the Majorana Hamiltonian (8) below by using the Jordan-Wigner transformation as follows. Referring to Refs. 29–32, we first introduce a fermion operator \( a_{iJ} \) at the site \( (\ell, m) \) such that the Pauli matrices are represented as

\[
\sigma_{\ell,m}^+ = 2a_{(\ell,m)}e^{i\pi\gamma_{\ell,m}},
\]

\[
\sigma_{\ell,m}^- = 2e^{i\pi\gamma_{\ell,m}}a_{\ell,m}^\dagger,
\]

\[
\sigma_{\ell,m}^z = (-1)^\ell \left[ 2a_{\ell,m}^\dagger a_{\ell,m} - 1 \right],
\]

where \( \sigma_{\ell,m}^\pm = \sigma_{\ell,m}^x \pm i\sigma_{\ell,m}^y \), and

\[
\hat{\theta}_{\ell,m} = \sum_{m' < m} 2L_x \sum_{\ell' < \ell} a_{\ell',m'}^\dagger a_{\ell',m'} + \sum_{\ell' < \ell} a_{\ell,m}^\dagger a_{\ell,m}.
\]

Further, by introducing the Majorana fermions, \( c_i \) and \( d_i \), as [29–32]

\[
c_{\ell,m} = i \left[ a_{\ell,m}^\dagger - a_{\ell,m} \right],
\]

\[
d_{\ell,m} = a_{\ell,m}^\dagger + a_{\ell,m} \quad \text{if } \ell \text{ is odd},
\]

and

\[
c_{\ell,m} = a_{\ell,m}^\dagger + a_{\ell,m},
\]

\[
d_{\ell,m} = i \left[ a_{\ell,m}^\dagger - a_{\ell,m} \right] \quad \text{if } \ell \text{ is even},
\]

the Hamiltonian of Eq. (1) can be written as

\[
H = iJ_x \sum_{\ell=1}^{L_x} \sum_{m=1}^{L_y} c_{(\ell-1,m)}^\dagger c_{(\ell,m)} + iJ_y \sum_{\ell=1}^{L_x-1} \sum_{m=1}^{L_y-1} c_{(\ell,m)}^\dagger c_{(\ell+1,m)} + J_z \sum_{\ell=1}^{L_x} \sum_{m=1}^{L_y} c_{(\ell,m)}^\dagger d_{(\ell,m)} d_{(\ell-1,m+1)}.
\]

Since any pairs of \( z \)-bonds do not share a site, \( d_{(\ell,m)}^\dagger d_{(\ell-1,m+1)} \) commute with the Hamiltonian. This allows us to replace this operator with the c-number

II. KITAEV HONEYCOMB MODEL AND JORDAN-WIGNER TRANSFORMATION

We consider the spin-1/2 Kitaev magnet on the honeycomb lattice. The Hamiltonian is given by

\[
H = \sum_{\gamma \in \{x,y,z\}} \sum_{\langle i,j \rangle \in B_{\gamma}} J_{\gamma} \sigma_i^\gamma \sigma_j^\gamma,
\]

where \( \sigma_i^\gamma \) is the \( \gamma \) component of the Pauli matrices for \( \gamma = x, y, z \) at the site \( i \) in the honeycomb lattice shown in Fig. 1, and \( B_{\gamma} \) is the set of all the bonds \( \langle i,j \rangle \) (pairs of nearest neighbor two sites \( i, j \) in the honeycomb lattice) with the type \( \gamma \) whose three types, \( x, y, z \), are, respectively, denoted by three colors, red, blue and green, in Fig. 1; \( J_{\gamma} \) is the corresponding exchange integral which is a real parameter. We impose the open boundary condition in the horizontal direction and the periodic
\(d_{(2\ell,m)}d_{(2\ell-1,m+1)} = \pm i\), which acts as a phase factor leads to an effective flux for itinerant c-Majorana fermions. For the system on the torus, Lieb’s theorem ensures that the ground state is obtained when the flux configuration is uniform [33]. Clearly, the uniform flux can be realized by setting all the eigenvalues of \(d_{(2\ell,m)}d_{(2\ell-1,m+1)}\) to be the same for a given \(m\) [29]. For the cylinder geometry which we consider here, we have numerically confirmed that the ground state is obtained in the same configuration of the eigenvalue of \(d_{(2\ell,m)}d_{(2\ell-1,m+1)}\). In the following, we set \(d_{(2\ell,m)}d_{(2\ell-1,m+1)} = +i\) for every \((\ell, m)\), and we represent the corresponding wavefunction as \(|\Phi^{(0)}_{\text{flux}}\rangle\).

In this case, the Hamiltonian is written in terms of the

\[
H = J_x \sum_{\ell=1}^{L_x} \sum_{m=1}^{L_y} \left[ \alpha_{(\ell,m)}^\dagger \alpha_{(\ell,m)} - \alpha_{(\ell,m)} \alpha_{(\ell,m)}^\dagger \right] + J_y \sum_{\ell=1}^{L_x-1} \sum_{m=1}^{L_y} \left[ \alpha_{(\ell,m)} \alpha_{(\ell+1,m)} - \alpha_{(\ell,m)}^\dagger \alpha_{(\ell+1,m)}^\dagger \right] + J_z \sum_{\ell=1}^{L_x} \sum_{m=1}^{L_y} \left[ \alpha_{(\ell,m)} \alpha_{(\ell,m+1)} \right. \\
\left. - \alpha_{(\ell,m)}^\dagger \alpha_{(\ell,m+1)} \right] .
\]

Further, we write \(\tilde{\alpha}_i = \alpha_i\) and \(\tilde{\alpha}_i^\dagger = \alpha_i^\dagger\) with \(i = (\ell, m)\). Also, for the superscript \(\zeta = \pm\) of the new fermion operators, we define \(\tilde{\zeta}\) as \(\tilde{\zeta} = -\) if \(\zeta = +\) and \(\tilde{\zeta} = +\) if \(\zeta = -\). Then, the Hamiltonian can be written in the form,

\[
H = \sum_{\zeta, \eta = \pm} \sum_{i,j} \tilde{\alpha}^\zeta_i \mathcal{H}_{ij} \tilde{\alpha}^\eta_j ,
\]

where \(\mathcal{H}\) is the complex-valued matrix, i.e., the single-body Hamiltonian. Let \(\varphi\) be a single-body wavefunction whose components are given by \(\varphi_i^\zeta\) with \(i = (\ell, m)\). The explicit action of the Hamiltonian \(\mathcal{H}\) for the wavefunction \(\varphi\) is written as

\[
(\mathcal{H}\varphi)(\ell,m) = J_x \tau^x \varphi(\ell,m) \\
- J_y \tau^y \varphi(\ell-1,m) - J_z \tau^z \varphi(\ell+1,m) \\
- J_y \tau^y \varphi(\ell,m-1) - J_z \tau^z \varphi(\ell,m+1) ,
\]

where \(\tau^\gamma\) is the \(\gamma\) component of the Pauli matrices which act on the internal degree of freedom denoted by the superscript \(\zeta = \pm\).

The form in Eq. (13) enables us to find simple forms of the symmetry operations. Firstly, it is invariant under the time reversal transformation given by the simple complex conjugate, since the Hamiltonian \(\mathcal{H}\) is real symmetric. Secondly, under the transformation given by \(\tau^\tau\), the Hamiltonian \(\mathcal{H}\) changes its sign. Thus, it has the chiral symmetry, too. Finally, as is well known, the combination of time reversal and chiral symmetries gives the particle-hole symmetry. In consequence, the classification class of the Hamiltonian as a topological material is BDI class [34–36]. The topological invariant is an integer-valued winding number for the system on the infinity-long strip. Further, if this number is nonvanishing, then there appears an edge zero mode in the system with an edge by virtue of the bulk-edge correspondence,
as we will see in the next section.

III. MAJORANA EDGE FLAT BAND IN $A_y$ PHASE

A. Solution of BdG equation in momentum space

Using the Fourier transform in the vertical direction,

$$\alpha_{\ell,k_y} = \sum_{m=1}^{L_y} e^{ik_y m} \alpha_{(\ell,m)},$$

we obtain the BdG form of the Hamiltonian in the momentum space:

$$H = \sum_{k_y} \Psi^\dagger(k_y) \hat{h}(k_y) \Psi(k_y),$$

where

$$\Psi(k_y) = (\alpha_{1,k_y}, \cdots, \alpha_{L_x,k_y}, \alpha_{1,-k_y}, \cdots, \alpha_{L_x,-k_y})^T,$$

and

$$\hat{h}(k_y) = \begin{pmatrix} \hat{h}_0(k_y) & \hat{\Delta}(k_y) \\ \hat{\Delta}^\dagger(k_y) & -\hat{h}_0(-k_y) \end{pmatrix},$$

with

$$[\hat{h}_0(k_y)]_{\ell,\ell'} = J_x - J_z \cos k_y \delta_{\ell,\ell'} - \frac{J_y}{2} (\delta_{\ell,\ell'-1} + \delta_{\ell,\ell'+1}).$$

$$[\hat{\Delta}(k_y)]_{\ell,\ell'} = -i J_z \sin k_y \delta_{\ell,\ell'} - \frac{J_y}{2} (\delta_{\ell,\ell'-1} - \delta_{\ell,\ell'+1}).$$

The energy spectra for four different phases [1] are shown in Fig. 2. Among four phases, B phase has gapless spectrum in a bulk and the flat band with zero energy at the edges. Only $A_y$ phase shows both of the gapped spectrum in the bulk and the flat band with zero energy at the edges for the present geometry of the edges. This is associated with the topological nature of the Hamiltonian of Eq. (15).

The origin of the zero energy modes can be understood by considering the special case. Namely, let us assume that $J_z = 0$. Then, the model becomes the independent $L_y$ chains. For a large $J_y$, each chain shows the winding number 1. Therefore, the $L_y$ chains give the total winding number $L_y$ due to the additivity of the index. As is well known, the homotopy argument guarantees that when varying the model parameters continuously, i.e., restoring the interchain coupling $J_z$, the topological invariant, or the winding number, does not change as long as the spectral or mobility gap of the Hamiltonian does not close. Thus, the winding number always takes the value $L_y$ in the whole regime $A_y$. Due to the bulk-edge correspondence, this implies that there appear zero energy edge modes whose number is at least $L_y$ (per edge). This is nothing but a flat edge band.

In the following, we consider $A_y$ phase, and derive the wave function of zero-energy modes by directly solving the BdG equation. Since the zero modes are doubly-degenerate at each $k_y$, we label them as $\gamma^{(\nu)}_{k_y}$, $\nu = 1,2$. Each zero mode can be expanded by $\alpha$ of (10) as

$$\gamma^{(\nu)}_{k_y} = \sum_{\ell=1}^{L_y} u^{(\nu)}_{\ell,k_y} \alpha_{\ell,k_y} + v^{(\nu)}_{\ell,k_y} \alpha^\dagger_{\ell,-k_y},$$

with the coefficients, $u^{(\nu)}_{\ell,k_y}$ and $v^{(\nu)}_{\ell,k_y}$. The energy eigenvalue equation of the coefficients, $u^{(\nu)}_{\ell,k_y}$ and $v^{(\nu)}_{\ell,k_y}$, at zero energy is given by

$$\begin{pmatrix} u^{(\nu)}_{1,k_y} \\ \vdots \\ u^{(\nu)}_{L_y,k_y} \\ v^{(\nu)}_{1,k_y} \\ \vdots \\ v^{(\nu)}_{L_y,k_y} \end{pmatrix} = 0.$$  

From Eqs. (18) and (19), Eq. (21) can be rewritten as

$$K_1 u^{(\nu)}_{\ell,k_y} - K_2 v^{(\nu)}_{\ell,k_y} = -\frac{J_y}{2} (u^{(\nu)}_{\ell-1,k_y} - v^{(\nu)}_{\ell-1,k_y}) - \frac{J_y}{2} (u^{(\nu)}_{\ell+1,k_y} + v^{(\nu)}_{\ell+1,k_y}) = 0.$$ 

FIG. 2. (a) The phase diagram of the Kitaev honeycomb model with $J_x + J_y + J_z = 1$. (b)-(e) Dispersion relations of itinerant Majorana fermions for (b) B phase, (c) $A_x$ phase, (d) $A_y$ phase, and (e) $A_z$ phase.

PHASE

A. Solution of BdG equation in momentum space
\[-K_1 v_{\ell,k_y}^{(\nu)} + K_2 u_{\ell,k_y}^{(\nu)} - \frac{J_y}{2} (u_{\ell-1,k_y}^{(\nu)} - v_{\ell-1,k_y}^{(\nu)}) + \frac{J_y}{2} (u_{\ell+1,k_y}^{(\nu)} + v_{\ell+1,k_y}^{(\nu)}) = 0, \tag{23}\]

where $K_1 = J_x - J_z \cos k_y$, and $K_2 = iJ_z \sin k_y$. To solve this, we introduce $s_{\ell,k_y}^{(\nu)} \equiv u_{\ell,k_y}^{(\nu)} - v_{\ell,k_y}^{(\nu)}$ and $\zeta_{\ell,k_y}^{(\nu)} \equiv u_{\ell,k_y}^{(\nu)} + v_{\ell,k_y}^{(\nu)}$. By adding and subtracting the two equations, (22) and (23), we obtain

\[
(K_1 + K_2)s_{\ell,k_y}^{(\nu)} - J_y s_{\ell-1,k_y}^{(\nu)} = 0, \tag{24}\]

and

\[
(K_1 - K_2)s_{\ell,k_y}^{(\nu)} - J_y s_{\ell+1,k_y}^{(\nu)} = 0. \tag{25}\]

Since we consider $A_y$ phase, i.e., a large $J_y$, we treat the case that the parameters of the Hamiltonian satisfy the condition,

\[
\left| \frac{K_1 \pm K_2}{J_y} \right| < 1, \tag{26}\]

or, equivalently,

\[
\sqrt{J_x^2 + J_z^2 - 2J_xJ_z \cos k_y} < |J_y|. \tag{27}\]

As we will see below, this condition is enough to find the edge zero modes [20]. Further, we consider the system with a sufficiently large length $L_x$ so that the exponential correction in the length $L_x$ can be ignored. Then, Eq. (24) has no left-edge solution because of the open boundary condition $\zeta_0 = 0$, but it has the right-edge solution,

\[
\zeta_{\ell,k_y}^{(1)} = \left( \frac{K_1 + K_2}{J_y} \right)^{L_x-\ell} \zeta_{L_x,k_y}^{(1)}. \tag{28}\]

Similarly, Eq. (25) has no right-edge solution by the boundary condition $\zeta_{L_x+1} = 0$, but it shows the left-edge solution,

\[
\zeta_{\ell,k_y}^{(2)} = \left( \frac{K_1 - K_2}{J_y} \right)^{\ell-1} \zeta_{1,k_y}^{(2)}. \tag{29}\]

Since all of $\zeta_{\ell,k_y}^{(2)}$ are vanishing for the latter case, i.e., the left-edge mode, we obtain

\[
u_{\ell,k_y}^{(2)} = \nu_{\ell,k_y}^{(2)} = \left( \frac{J_x - J_z \cos k_y}{J_y} \right)^{\ell-1} \frac{N(k_y)}{N(k_y)}, \tag{30}\]

where $N(k_y)$ is the normalization factor as a function of $k_y$.

### B. Wannier orbitals

The flatness of the Majorana edge band enables us to construct Wannier orbitals which are localized in the real-space. Namely, we define $\gamma_n^{(\nu)}$ as

\[
\gamma_n^{(\nu)} = \frac{1}{L_y} \sum_{k_y} e^{-ik_y m} n_{\ell,k_y}^{(\nu)} = \frac{1}{L_y} \sum_{k_y} e^{-ik_y n} \left( \sum_{\ell=1}^{L_x} u_{\ell,k_y}^{(\nu)} \alpha_{\ell,k_y} + v_{\ell,k_y}^{(\nu)} \alpha^\dagger_{\ell,-k_y} \right),
\]

\[
= \frac{1}{L_y} \sum_{k_y} e^{-ik_y n} \left\{ \sum_{\ell=1}^{L_x} \sum_{m=1}^{L_y} e^{ik_y m} \left( u_{\ell,k_y}^{(\nu)} \alpha_{\ell,m} + v_{\ell,k_y}^{(\nu)} \alpha^\dagger_{\ell,m} \right) \right\}. \tag{31}\]

Introducing the coefficients $U_n^{(\nu)}(\ell, m)$ and $V_n^{(\nu)}(\ell, m)$ as

\[
U_n^{(\nu)}(\ell, m) \equiv \frac{1}{L_y} \sum_{k_y} e^{ik_y (m-n)} u_{\ell,k_y}^{(\nu)}, \tag{32}\]

\[
V_n^{(\nu)}(\ell, m) \equiv \frac{1}{L_y} \sum_{k_y} e^{ik_y (m-n)} v_{\ell,k_y}^{(\nu)}, \tag{33}\]

$\gamma_n^{(\nu)}$ is written as

\[
\gamma_n^{(\nu)} = \sum_{\ell=1}^{L_x} \sum_{m=1}^{L_y} U_n^{(\nu)}(\ell, m) \alpha_{\ell,m} + V_n^{(\nu)}(\ell, m) \alpha^\dagger_{\ell,m}. \tag{34}\]

In the following, we will consider only the left edge mode, i.e., the case with $\nu = 2$, because we can deal with the case of the right edge mode in the same way. Clearly, from the condition $u_{\ell,k_y}^{(\nu)} = v_{\ell,k_y}^{(\nu)}$ in the case with $\nu = 2$ and the definitions, (32) and (33), of $U_n^{(2)}(\ell, m)$ and $V_n^{(2)}(\ell, m)$, one has $U_n^{(2)}(\ell, m) = V_n^{(2)}(\ell, m)$. Therefore, the Wannier function of (31) with $\nu = 2$ can be written as

\[
\gamma_n^{(2)} = \sum_{\ell=1}^{L_x} \sum_{m=1}^{L_y} U_n^{(2)}(\ell, m) [\alpha_{\ell,m} + \alpha^\dagger_{\ell,m}],
\]

\[
= \sum_{\ell=1}^{L_x} \sum_{m=1}^{L_y} U_n^{(2)}(\ell, m) c_{2\ell-1,m}. \tag{35}\]

where we have used the relation (10). From Eq. (32) and the explicit form (30) of $u_{\ell,k_y}^{(2)}$, one notices $U_n^{(2)}(\ell, m)$
FIG. 3. The absolute value of the coefficient $U_n^{(2)}(\ell, m)$ for (a) $n = 1$ and (b) $n = 2$ for the system with $L_x = L_y = 32$. (c) and (d) are for fixed $m$ to $m = 1$ and $m = 2$, respectively. Blue and orange lines denote $n = 1$ and $n = 2$, respectively. The exchange parameters used here are $(J_x, J_y, J_z) = (0.15, 0.7, 0.15)$.

is real. Therefore, $\gamma^{(2)}_n$ of (31) satisfies the Majorana condition, $[\gamma^{(2)}_n]^\dagger = \gamma^{(2)}_n$, i.e., it is a Majorana fermion. We choose the normalization factor $N(k_y)$ so that $\gamma^{(2)}_n$ satisfies $\{\gamma^{(2)}_n, \gamma^{(2)}_{n'}\} = 2\delta_{n,n'}$, which leads to

$$\sum_{\ell=1}^{L_x} \sum_{m=1}^{L_y} |U_n^{(2)}(\ell, m)|^2 = 1. \quad (36)$$

In Fig. 3, we show $|U_n^{(2)}(\ell, m)|$ for $n = 1$ and 2. We can see that the distribution of $|U_n^{(2)}(\ell, m)|$ is concentrated at $(\ell, m) = (1, n)$, and rapidly decays with the distance.

IV. EDGE MAGNETIZATION

Now we compute the edge magnetization at the left edge. More precisely, we calculate the expectation value $\frac{1}{L_y} \sum_{m=1}^{L_y} |\gamma^{(2)}_{1,m}\rangle$, $\gamma = x, y, z$, where $\langle O \rangle$ stands for the expectation value of the operator $O$ with respect to a ground state.

A. Warm-up: corner magnetization

Before calculating the edge magnetization, it is instructive to calculate the magnetization at the corner site, i.e., $(\ell, m) = (1, 1)$. The spin operators $\sigma^{(2)}_{1,1}$ are written in terms of the Majorana fermions, $c_i, d_i$, by using Eqs. (2)-(4) and Eq. (6), as

$$\sigma^{(2)}_{1,1} = d_{(1,1)}.$$  

Clearly, both of the two operators, $\sigma^{(1,1)}_x$ and $\sigma^{(1,1)}_y$, contain the single Majorana fermion $d_{(1,1)}$. We recall the well-known fact [29–32] that the gauge-field sector of the ground state is the eigenstate of pairs of the d-Majorana fermions, $d_{(2\ell,m)}d_{(2\ell+1,m)}$, whose eigenvalue acts as an effective phase for the itinerant c-Majorana fermions. This fact also means that the fermion parity of the d-Majorana fermions is a good quantum number. Combining these observations with the fact that the ground state has a uniform flux, one notices that a Majorana excitation created by an odd number of the operators $d_i$ above the ground state is gapped in the present $A_y$ phase. This implies that the expectation values of $\sigma^{(1,1)}_x$ and $\sigma^{(1,1)}_y$ with respect to the ground state must be vanishing. On the other hand, the Majorana operator $c_{(1,1)}$ in the right-hand side of Eq. (38) creates a Majorana edge zero mode above a ground state as we will see in Eq. (41) below. Therefore, we can expect that only the expectation value of $\sigma^{(1,1)}_z$ is nonvanishing. We note that the vanishing of the expectation value for $x$- and $z$-components occurs for arbitrary $(1, m)$ with $m = 2, 3, \ldots$, thus the entire edge magnetization also shows the unidirectional nature.

To calculate the expectation value of $\sigma^{(1,1)}_z$ with respect to a ground-state vector, we recall that the ground state of the c-Majorana fermion sector is degenerate due to the zero modes which form the flat band at the edge. Let us consider a form of the ground state which is given by

$$|\text{GS}_c\rangle = (s + t\gamma^{(2)}_1)\left|0, \Phi^{(0)}_{\text{flux}}\right\rangle,$$  

where the complex numbers, $s$ and $t$, satisfy $|s|^2 + |t|^2 = 1$ for the normalization $\langle \text{GS}_c | \text{GS}_c \rangle = 1$, and $\left|0, \Phi^{(0)}_{\text{flux}}\right\rangle$ is the total ground state including the flux sector for d-Majorana fermions, whose negative energy levels are all occupied by the usual complex fermions which diagonalize the Hamiltonian. Then, the expectation value of $\sigma^{(1,1)}_z$ with respect to $|\text{GS}_c\rangle$ is written as

$$\langle \text{GS}_c | \sigma^{(1,1)}_z | \text{GS}_c \rangle = \langle 0 | (s^* + t^*\gamma^{(2)}_1) c_{(1,1)} (s + t\gamma^{(2)}_1) | 0 \rangle.$$  

In order to calculate this right-hand side, we expand the operator $c_{(1,m)}$ in terms of the fermions which diagonalize the Hamiltonian as

$$c_{(1,m)} = W^{m}_{1}\gamma^{(2)}_1 + W^{m}_{2}\gamma^{(2)}_2 + \ldots + W^{m}_{L_y}\gamma^{(2)}_{L_y} + \ldots,$$  

where we have written $\gamma^{(2)}_n$ terms only because the rest of the terms do not contribute to the magnetization as we will show below. The coefficients $W^m_n$ are determined by the anticommutator with $\gamma^{(2)}_n$, i.e.,

$$\{\gamma^{(2)}_n, c_{(1,m)}\} = 2W^m_n.$$
On the other hand, from Eq. (35), we have
\[ \{ c_{1,m}, \gamma_n^{(2)} \} = 2U_n^{(2)}(1, m). \quad (44) \]

Combining these equations, we have
\[
c_{1,m} = U_1^{(2)}(1, m)\gamma_1^{(2)} + U_2^{(2)}(1, m)\gamma_2^{(2)} + \ldots + U_{L_x}^{(2)}(1, m)\gamma_{L_x}^{(2)} + \ldots
\]
\[ = \langle \text{max} \rangle \]

Substituting (45) with \( m = 1 \) into (41), we obtain
\[
\langle G_S | \sigma^y_{(1,1)} | G_S \rangle = (s^t + st^*)U_1^{(2)}(1, 1), \quad (46)
\]
where we have used the anticommutativity and the normalization \( (\gamma_1^{(2)})^2 = 1 \) for \( \gamma_1^{(2)} \), and the fermion parity conservation for \( |0\rangle \).

The present result (46) implies that, if we apply an infinitesimally weak magnetic field in the \( y \)-direction at the site \((1, 1)\), the magnetization \( \langle G_S | \sigma^y_{(1,1)} | G_S \rangle \) is maximized so as to gain the maximum Zeeman energy. Thus, we have to determine the coefficients \( s \) and \( t \) so that the magnetization is maximized. We can easily find its maximum value by choosing \( s = t = \frac{1}{\sqrt{2}} \) (up to the overall phase factor), as
\[
\langle G_S | \sigma^y_{(1,1)} | G_S \rangle = U_{1,1}^{(2)}(1).
\]

From this result, we see that, from the expression (35) of \( \gamma_{n}^{(2)} \) in terms of \( c_{(2L-1,m)} \), the value of the corner magnetization is given by the amplitude of the Majorana fermion \( c_{(1,1)} \) in the Wannier orbital \( \gamma_1^{(2)} \). Another key observation is that we need a linear combination of \( |0\rangle \) and \( |\gamma_1^{(2)}\rangle \), namely the fermion parity of \( e \)-Majorana fermion has to be mixed, to obtain a finite magnetization, since the spin operator has an odd parity of \( e \)-Majorana fermion.

**B. Edge magnetization**

Keeping these observations in mind, we move on to the calculation of the entire edge magnetization. To do this, we have to calculate the expectation value \( \langle \gamma_{(1,m)} \rangle \) with arbitrary \( m \). Again, from Eqs. (2)-(4) and Eq. (6), we obtain the Majorana representation of the spin operator:
\[
\sigma^y_{(1,m)} = c_{(1,m)}e^{i\hat{\theta}_{(1,m)}}.
\]

From Eq. (48), we see that we now have to deal with the non-local operator \( e^{i\hat{\theta}_{(1,m)}} \), which is the *total* fermion parity operator (i.e., the fermion parity for both \( e \)- and \( d \)-Majorana fermions) below \( m \)-th row.

What wavefunction do we need to choose to obtain the finite expectation value for all \( m = 1, 2, \ldots, L_y \)? To see this, let us consider a trial wavefunction,
\[
\langle G_S | = 2^{-\frac{L_y}{2}}S[(1 + \Gamma_1)(1 + \Gamma_2) \cdots (1 + \Gamma_{L_y})]|0, \Phi_{\text{flux}}^{(0)}\rangle,
\]
where
\[
\Gamma_n = e^{i\theta_n^{(1,n)}}, \quad (50)
\]
for \( n = 1, 2, \ldots, L_y \), and \( S[\cdots] \) is the spatially ordered product which is defined as follows:
\[
S[\Gamma_1, \Gamma_2, \ldots, \Gamma_{L_y}] = e^{i\hat{\theta}_{(1,r_1)}}e^{i\hat{\theta}_{(1,r_2)}} \cdots e^{i\hat{\theta}_{(1,r_{L_y})}} \times \gamma_{r_1}^{(2)} \gamma_{r_2}^{(2)} \cdots \gamma_{r_{L_y}}^{(2)}|0, \Phi_{\text{flux}}^{(0)}\rangle.
\]

For \( r_1, r_2, \ldots, r_N \) satisfying \( r_1 < r_2 < \cdots < r_N \). Although the form of the wavefunction in Eq. (49) is seemingly complicated, one can see that this is a natural extension of \( |G_S\rangle \), namely, the factor \( \frac{1}{\sqrt{2}}(1 + \gamma_1^{(2)}) \) is replaced with a product over the entire edge, \( S[\prod_{n=1}^{L_y} \frac{1}{\sqrt{2}}(1 + \Gamma_n)] \). However, there are two sharp differences between (40) and (49). Firstly, the expression of (49) includes not only \( \gamma_n^{(2)} \) but also \( e^{i\hat{\theta}_{(1,n)}} \). Since \( e^{i\hat{\theta}_{(1,n)}} \) acts on both \( e \)-Majorana fermion sector and the flux sector, the flux part of \( G_S \) is no longer equal to the original one. Nevertheless, \( G_S \) is still a ground state of the Hamiltonian, as we will show below. Secondly, there is a spatial ordering operator in Eq. (49). Actually, thanks to the spacial ordering, we can show that \( G_S \) is indeed a ground state. To be more specific, one can show that \( e^{i\hat{\theta}_{(1,n)}} \) commute with the Hamiltonian, which means that for an arbitrary ground state of the Hamiltonian \( |GS\rangle \), \( e^{i\hat{\theta}_{(1,n)}} |GS\rangle \) is a ground state as well. Applying this to the terms in (49), we observe the following:
\[
\langle GS | c_{(1,m)}e^{i\hat{\theta}_{(1,m)}} | GS \rangle
\]
Let us proceed to the calculation of the expectation value \( \langle G_S | \sigma_{(1,m)} | G_S \rangle \). To perform this calculation, let us recall the fact that the operator \( e^{i\hat{\theta}_{(1,m)}} \) changes the fermion parity of a \( d \)-Majorana-fermion state for a bond belonging to \( B \). This leads to \( \langle \psi, \Phi_{\text{flux}}^{(0)} | e^{i\hat{\theta}_{(1,m)}} | \psi, \Phi_{\text{flux}}^{(0)} \rangle = 0 \) for an arbitrary choice of \( |\psi\rangle \) as a wavefunction in the \( c \)-fermion sector. Thus, the non-vanishing contributions in the expectation value are given by the terms,
\[
2^{-L_y} \langle 0, \Phi_{\text{flux}}^{(0)} | \gamma_{r_1}^{(2)} \cdots \gamma_{r_{L_y}}^{(2)} e^{i\hat{\theta}_{(1,r_1)}} \cdots e^{i\hat{\theta}_{(1,r_{L_y})}} | 0, \Phi_{\text{flux}}^{(0)} \rangle
\]
\[
\times c_{(1,m)} e^{i\hat{\theta}_{(1,m)}} 2^{-L_y} e^{i\hat{\theta}_{(1,r_1)}} e^{i\hat{\theta}_{(1,r_2)}} \cdots e^{i\hat{\theta}_{(1,r_{L_y})}} e^{i\hat{\theta}_{(1,r_{L_y})}} \cdots e^{i\hat{\theta}_{(1,r_{L_y})}} | 0, \Phi_{\text{flux}}^{(0)} \rangle,
\]
\[
(52)
\]
where \( r_p = m \). We note that \( \{ c_{(1,m)}, e^{i\pi \hat{h}_{(1,n)}} \} = 0 \) for \( m < n \) and \( \{ c_{(1,n)}, c_{(1,m)} \} = 0 \) for \( m \geq n \). These commutation relations are a consequence of the facts that the operator \( e^{i\pi \hat{h}_{(1,n)}} \) is the fermion parity below the \( n \)-th row and that the fermion operator \( c_{(1,m)} \) changes the fermion parity at the \( m \)-th row. Using these relations and the anticommutativity of \( \gamma_m^{(2)} \), the term of (52) can be written as

\[
2^{-L_y} \langle 0 | \gamma_{r_1}^{(2)} \gamma_{r_2}^{(2)} \cdots \gamma_{r_{p-1}}^{(2)} \gamma_{r_{p+1}}^{(2)} \cdots \gamma_{r_N}^{(2)} c_{(1,m)} \gamma_m^{(2)} \gamma_{r_N}^{(2)} \cdots \gamma_{r_{p-1}}^{(2)} \gamma_{r_{p+1}}^{(2)} \cdots \gamma_{r_2}^{(2)} \gamma_{r_1}^{(2)} | 0 \rangle. \tag{53}
\]

By adding the conjugate contribution, we have

\[
2^{-L_y} \langle 0 | \gamma_{r_1}^{(2)} \gamma_{r_2}^{(2)} \cdots \gamma_{r_{p-1}}^{(2)} \gamma_{r_{p+1}}^{(2)} \cdots \gamma_{r_N}^{(2)} c_{(1,m)} \gamma_m^{(2)} \gamma_{r_N}^{(2)} \cdots \gamma_{r_{p-1}}^{(2)} \gamma_{r_{p+1}}^{(2)} \cdots \gamma_{r_2}^{(2)} \gamma_{r_1}^{(2)} | 0 \rangle. \tag{54}
\]

From (44), we find that the anticommutator in (54) is equal to \( 2U_m^{(2)}(1,m) \). Therefore, the corresponding contribution becomes \( 2U_m^{(2)}(1,m) \). Recalling the fact that there are \( 2^{L_y-1} \) choices of such \( r_1 \cdots r_N \) (notice that one of the \( r_1 \cdots r_N \) has to be equal to \( m \)), we obtain \( \langle \text{GS}_e | \sigma^{(2)}_{(1,m)} | \text{GS}_e \rangle = U_m^{(2)}(1,m) \). In the same way, one can also show that \( \langle \text{GS}_e | \text{GS}_e \rangle = 1 \). Consequently, we have

\[
\frac{1}{L_y} \sum_{m=1}^{L_y} \langle \text{GS}_e | \sigma^{(2)}_{(1,m)} | \text{GS}_e \rangle = \frac{1}{L_y} \sum_{m=1}^{L_y} U_m^{(2)}(1,m) = U_1^{(2)}(1,1) \tag{55}
\]

To obtain the final line of (55), we use the relation \( U_m^{(2)}(1,m) = U_1^{(2)}(1,1) \) which can be derived from (32). We remark that, although we can not exclude the possibility that there is an alternative choice of the ground state having a larger edge magnetization than that for \( | \text{GS}_e \rangle \), the present result of (55) provides the lower bound of the edge magnetization under the infinitesimally small external magnetic field.

In Fig. 4, we plot the parameter dependence of the magnetization in \( \Lambda_y \) phase. It takes the maximum value 1 for \( (J_x, J_y, J_z) = (0, 1, 0) \), since the edge spins completely behave as usual free spins in this limit. As the values of the parameters, \( J_x, J_y, J_z \), approach the phase boundary, the magnetization decreases to a small value.

\[ \text{FIG. 4. The } y\text{-component of the edge magnetization (per site) as a function of } (J_x, J_y, J_z) \text{ in } \Lambda_y \text{ phase. The system size used for the numerical calculation is } L_z = L_y = 32. \]

### V. DISCUSSIONS

#### A. Stability of edge magnetization

We first address the stability of the edge magnetization against perturbations such as disorder and additional interactions.
site $i$ on a honeycomb lattice, we can construct the edge zero mode (for details, see Appendix B).

When a perturbation is an interaction between fermions which cannot be mapped to a free-fermion form, the Hamiltonian cannot be diagonalized in terms of Majorana fermions in general. Actually, if we introduce a standard Heisenberg interaction into the Kitaev spin Hamiltonian, then a pair of $d$-Majorana fermions on $z$-bonds is no longer conserved. It is a highly nontrivial problem whether or not the edge zero modes still survive under such a perturbation. Since the free-fermion picture does not work well in this situation, we recall the valence bond picture, or, the idea of paired and unpaired fermions. Consider the situation that all the couplings for $y$ bonds are very strong compared to the other couplings. Then, we can expect that the internal degrees of freedom for all the pairs of two spins connected by $y$ bonds are frozen, and that there remains a possibility that only the spins at the edges are not frozen and behave as a free spin. However, clearly, if we introduce a direct interaction between the spins at the edges, then we cannot expect that the edge zero modes survive. What is the necessary condition that the edge zero modes survive? We recall that the present unperturbed Kitaev Hamiltonian has time-reversal and particle-hole symmetries. Roughly speaking, these symmetries protect the edge flat band against perturbations. If the excitations of the quasi-particles near zero energy effectively preserve these symmetries under the additional interactions, then, we can expect that the edge flat band is not destroyed, as long as the bulk energy gap does not collapse, i.e., the system remains in a gapped spin liquid phase.

**B. Comparison with related works**

We briefly comment on related works. In the Kitaev model with site vacancy, localized zero energy states were found near the vacancy sites [37, 38], and these states yield a similar local magnetization to those in the present paper. For the $SU(2)$-symmetric version of the Kitaev model [39], an edge magnetization was obtained recently. This edge magnetization also comes from the localized zero energy states. Thus, the appearance of the local magnetization is ubiquitous in the Kitaev-type models. Needless to say, in many models, various kinds of topological boundary states such as chiral edge modes [30] and corner modes [40] have been found to appear.

In the present paper, we have clarified the topological origin of the Majorana edge flat band which yields the edge magnetization by relying on the bulk-edge correspondence from the weak topological point of view. The advantage of this approach is that the stability of the Majorana edge flat band is guaranteed by the topological nature. This is very important from an experimental point of view because an additional perturbation such as disorder is often inevitable in experiments. However, we cannot explain the topological origin for all of the similar localized modes as in above by using our approach. Elucidating the topological origin of various boundary states is left for future studies.

**C. Measurement of edge magnetization in experiments**

Finally, we address the possible experimental setup to measure the edge magnetization. In the present Kitaev magnet, the highly anisotropic exchange integrals yield the large bulk gap above the ground state. Our result implies that the situation also leads to the large edge magnetization. Such a highly anisotropic magnet may be experimentally feasible by applying a pressure to the Kitaev-magnet candidates [41]. But the additional interactions, such as the Heisenberg interaction, are also enhanced by the pressure. Hence, it would be desirable to seek the novel materials having the bond-anisotropic Kitaev interactions to see the edge magnetization. If such a material is found, the highly unidirectional magnetization is expected to be detected by applying a weak external magnetic field at one of the edges of the sample, as far as neither the Zeeman energy nor the thermal fluctuations exceed the flux gap in the gauge-field sector and the bulk band gap of the itinerant Majorana fermions. We also stress the following: As we have shown, this magnetization appears only at the edges because the bulk is in the gapped spin liquid phase. Namely, if the external magnetic field is sufficiently weak, then the contribution of the magnetization from the bulk region can be expected to be negligible.

**VI. SUMMARY**

In summary, we have shown that the fractionalization of spins into Majorana fermions leads to a unidirectional edge magnetization in the Kitaev honeycomb model in a gapped phase on a cylinder geometry. The nonvanishing magnetization in a specific direction comes from the degeneracy of the ground state caused by the Majorana edge flat band and the fermion parity conservation of localized Majorana fermions. Since the Majorana edge flat band is stable due to a weak topological nature of the BdG Hamiltonian, the resulting edge magnetization is stable against the symmetry-preserving perturbations including disorders. We hope that our results shed light on the new way to detect the Majorana fermions in the condensed matter systems.

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Appendix A: Bulk-edge correspondence in one dimension

In this Appendix, we present a proof of the bulk-edge correspondence in one-dimensional tight-binding model for all the classes which show a topologically nontrivial index. Here the bulk-edge correspondence means the equality of the bulk index (\(\text{Ind}_B\)) and the edge index (\(\text{Ind}_E\)), defined below.

We begin our discussion with AIII, BDI, and CII classes, where the system has chiral symmetry, and topological phases are characterized by the winding number. For these classes, the proof has already been given by previous works [42, 43]. Here we give a proof that is slightly different from theirs. Note that the Kitaev honeycomb model, which belongs to BDI class, indeed has zero-energy edge modes whose number is equal to the bulk winding number, as we have seen in the main text.

We also prove of the bulk-edge correspondence for D and DIII classes which are characterized by a \(\mathbb{Z}_2\) index. As far as we know, the proof for these cases is new, although the proof is slightly similar to that for AIII, BDI, and CII classes having a \(\mathbb{Z}\) index.

1. AIII, BDI and CII Classes

We first consider AIII, BDI and CII classes characterized by the winding number. In the following, we denote by \(O^*\) the adjoint of the operator \(O\).

Let \(S\) be the chiral operator which satisfies \(S^2 = 1\) and \(S^* = S\). Then, the chiral symmetric bulk Hamiltonian \(H\) satisfies

\[
SHS = -H. \tag{A1}
\]

We assume that the hopping amplitudes of the tight-binding model are of finite range. Further, we require the following two assumptions:

- The energy \(E = 0\) is not an eigenvalue of the Hamiltonian \(H\).
- The energy \(E = 0\) is in the spectral gap of the Hamiltonian \(H\) or in the localization regime. More precisely, we assume that the resolvent exponentially decays with distance as

\[
\sup_{\varepsilon > 0} \|\chi_x(i\varepsilon - H)^{-1}\chi_y\| \leq C_0 \exp[-|x - y|/\xi_0], \tag{A2}
\]

where \(\chi_x\) is the characteristic function of the site \(x\), and the two positive constants, \(C_0\) and \(\xi_0\), depend only on the parameters of the tight-binding model.

We write \(P_\pm\) for the spectral projections onto the positive and negative energies, respectively. We also write

\[
\mathcal{U} := P_+ - P_- \tag{A3}
\]

for the flattened Hamiltonian, and its eigenvalue is \(+1\) (\(-1\)) if the corresponding eigenvalue of \(H\) is positive (negative). Clearly, one has \(S\mathcal{U}S = -\mathcal{U}\), and

\[
\mathcal{U} = \begin{pmatrix} 0 & \mathcal{U}_- \\ \mathcal{U}_+ & 0 \end{pmatrix}, \tag{A4}
\]

in the basis which diagonalizes the chiral operator \(S\) as

\[
S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{A5}
\]

One notices that the relation, \(\mathcal{U}_+ = (\mathcal{U}_-)\ast\), holds.

Next, to discuss the bulk-edge correspondence, we need to define the edge Hamiltonian \(H_E\) from the bulk Hamiltonian \(H\). To do this, we consider the half infinite chain with an open boundary at the left edge, and we introduce the projection operator \(\mathcal{P}\) which restricts the whole infinite chain into the half one so that the edge Hamiltonian \(H_E\) is given by

\[
H_E = \mathcal{P}HP. \tag{A6}
\]

Clearly, this projection operator \(\mathcal{P}\) is equal to the step or switch function whose support is the half chain. Therefore, the commutator, \(J := i[H, \mathcal{P}]\), that is an operator on the whole chain, is the current operator across the left edge of the half chain. We assume that the chiral operator \(S\) commutes with the projection operator \(\mathcal{P}\), i.e., \([S, \mathcal{P}] = 0\). When the chiral operator \(S\) acts on the internal degrees of freedom at each site, this condition is obviously fulfilled.

From (A1) and (A5), the Hamiltonian \(H\) can be written in the form

\[
H = \begin{pmatrix} 0 & H_- \\ H_+ & 0 \end{pmatrix}, \tag{A7}
\]

with \(H_- = (H_+)\ast\). One may also write \(H = \tilde{H}_+ + \tilde{H}_-\) with \(\tilde{H}_\pm = H \cdot \frac{1}{2}(1 \pm S)\). Then, the edge Hamiltonian \(H_E\) of (A6) can be written as

\[
H_E = \mathcal{P}\tilde{H}_+\mathcal{P} + \mathcal{P}\tilde{H}_-\mathcal{P}. \tag{A8}
\]

One notices that there are two types of zero modes. One is a set of eigenvectors of the chiral operator \(S\) with eigenvalue \(+1\). The other is that with the opposite eigenvalue \(-1\). The integer-valued index of the edge zero modes is defined by

\[
\text{Ind}_E := \text{Ind}(\mathcal{P}H_+\mathcal{P} + 1 - \mathcal{P}) \nonumber = \text{dim ker } (\mathcal{P}H_+\mathcal{P} + 1 - \mathcal{P}) \nonumber - \text{dim ker } (\mathcal{P}H_-\mathcal{P} + 1 - \mathcal{P}), \tag{A9}
\]

where \(\text{dim ker } (O)\) stands for the dimension of the kernel of an operator \(O\). Namely, the edge index, \(\text{Ind}_E\), is defined by the difference between the numbers of the two types of the edge states. In general, when an operator \(T\) satisfies \(\text{dim ker } (T) < \infty\) and \(\text{dim ker } (T\ast) < \infty\), the operator \(T\) is called the Fredholm operator [46, 47], and the
Fredholm index is defined by $\text{Ind} (T) := \text{dim ker} (T) - \text{dim ker} (T^*)$. In the following, the edge index $\text{Ind}_E$ will prove to be the Fredholm index.

In order to show that the edge index is equal to the bulk index, i.e., the winding number, we recall some results in Ref. 44. The bulk index is defined by

$$\text{Ind}_B := \frac{1}{2} \text{Tr} \left[ S (\mathcal{P} - u \mathcal{P} u) \right]. \quad (A10)$$

By using the supersymmetric structure [45] in the operator algebra, this index can be written as

$$\text{Ind}_B = \text{dim ker} (\mathcal{P} \mathcal{U}_+ \mathcal{P} + 1 - \mathcal{P})
\quad - \quad \text{dim ker} (\mathcal{P} \mathcal{U}_+ \mathcal{P} + 1 - \mathcal{P}). \quad (A11)$$

Thus, the bulk index $\text{Ind}_B$ takes an integer value.

The right-hand side of the bulk index (A10) can also be written in the form of the winding number as

$$\text{Ind}_B = \frac{1}{2 \pi i} \oint dz \text{Tr} \left[ S \frac{1}{z - H} J \frac{1}{z - H} \right]. \quad (A12)$$

In Eq. (A12), the contour integral in the complex plane is chosen so that the contour integral of the resolvent $(z - H)^{-1}$ yields the projection $P_-$ onto the sector of the negative energies of the Hamiltonian (see Fig. 6), i.e.,

$$P_- = \frac{1}{2 \pi i} \oint dz \frac{1}{z - H}. \quad (A13)$$

The projection $\mathcal{P}$ onto the half chain is equal to the characteristic function of the half chain. Combining this with the assumption that the hopping amplitudes of the tight-binding model are of finite range, one notices that the current operator $J$ has a finite support. Besides, from the assumption that the resolvent $(z - H)^{-1}$ has the upper bound that exponentially decays with distance at the Fermi level $E = 0$, the operator $(z - H)^{-1} J (z - H)^{-1}$ is trace class. Thus, the right-hand side of (A12) is well defined.

The proof of the equality of the bulk index (A10) and the winding number (A12) is as follows: Note that

$$\mathcal{P} - u \mathcal{P} u = \mathcal{U} [\mathcal{U}, \mathcal{P}] = -2 i (\mathcal{P} - \mathcal{P}_-), \quad (A14)$$

where we have used $\mathcal{U}^2 = 1$ and $\mathcal{U} = 1 - 2 \mathcal{P}_-$. The commutator in the right-hand side of (A14) is written

$$[\mathcal{P}_-, \mathcal{P}] = \frac{1}{2 \pi i} \oint dz \frac{1}{z - H} \mathcal{H} \frac{1}{z - H}
\quad = \frac{1}{2 \pi i} \oint dz \frac{1}{z - H} J \frac{1}{z - H}. \quad (A15)$$

where we have used the expression (A13) of the projection $P_-$, and $J = i [\mathcal{H}, \mathcal{P}]$. Substituting these into the right-hand side of (A10), one obtains the desired result (A12).

Now, we give a proof of the bulk-edge correspondence, i.e., $\text{Ind}_E = \text{Ind}_B$. The operator $H_+$ is the restriction of the Hamiltonian $\mathcal{H}$ onto the sector $\mathcal{H}_+$ with eigenvalue +1 for the chiral operator $S$, i.e.,

$$H_+ = H - \frac{1}{2} (1 + S) \bigg|_{\mathcal{H}_+}. \quad (A16)$$

Note that $H = |\mathcal{H}| \mathcal{U}$, where $|\mathcal{H}| = \sqrt{H^2}$. Using this polar decomposition, one has

$$\mathcal{P} H_+ \mathcal{P} = \mathcal{P} [H^2] \mathcal{P} |_{\mathcal{H}_+}
\quad = \mathcal{P} [H^2] \mathcal{P} |_{\mathcal{H}_+} + \mathcal{P}[H] (1 - \mathcal{P}) \mathcal{U} \mathcal{P} |_{\mathcal{H}_+}
\quad = \mathcal{P} [H] |_{\mathcal{H}_+} \mathcal{P} \mathcal{U} \mathcal{P} + \mathcal{P}[H] (1 - \mathcal{P}) \mathcal{U} \mathcal{P} |_{\mathcal{H}_+}. \quad (A17)$$

In order to treat the first term in the right-hand side of (A17), we recall the well known fact about Fredholm indices. (See, e.g., Refs. 46 and 47.) Let $T_1$ and $T_2$ be two Fredholm operators for which the product $T_1 T_2$ is defined. Then, the product $T_1 T_2$ is also the Fredholm operator, and the index satisfies the relation,

$$\text{Ind} (T_1 T_2) = \text{Ind} (T_1) + \text{Ind} (T_2). \quad (A18)$$

Note that

$$(\mathcal{P} [H] |_{\mathcal{H}_+} + 1 - \mathcal{P}) (\mathcal{P} \mathcal{U} \mathcal{P} + 1 - \mathcal{P})
\quad = \mathcal{P} [H] |_{\mathcal{H}_+} \mathcal{P} \mathcal{U} \mathcal{P} + 1 - \mathcal{P}. \quad (A19)$$

From the assumption of the spectrum of the Hamiltonian $\mathcal{H}$, one has $|\mathcal{H}| > 0$. Therefore, one obtains

$$\text{Ind} (\mathcal{P} [H] |_{\mathcal{H}_+} + 1 - \mathcal{P}) = 0. \quad (A20)$$

By using this and the relation (A18), we have

$$\text{Ind} (((\mathcal{P} [H] |_{\mathcal{H}_+} + 1 - \mathcal{P}) (\mathcal{P} \mathcal{U} \mathcal{P} + 1 - \mathcal{P}))
\quad = \text{Ind} (\mathcal{P} [H] |_{\mathcal{H}_+} + 1 - \mathcal{P}) + \text{Ind} (\mathcal{P} \mathcal{U} \mathcal{P} + 1 - \mathcal{P})
\quad = \text{Ind} (\mathcal{P} \mathcal{U} \mathcal{P} + 1 - \mathcal{P}). \quad (A21)$$
Combining this with the identity (A19), we obtain
\[ \text{Ind} (\mathcal{P}H\|_{\mathcal{P}} - \mathcal{P}\mathcal{U}_+\mathcal{P} + 1 - \mathcal{P}) = \text{Ind} (\mathcal{P}\mathcal{U}_+\mathcal{P} + 1 - \mathcal{P}). \] (A22)

Next, consider the second term in the right-hand side of (A17). As is well known, Fredholm indices are stable against a compact perturbation. Namely, for a Fredholm operator \( T \) and a compact operator \( K \), the following relation is valid: [46, 47]
\[ \text{Ind} (T + K) = \text{Ind} (T). \] (A23)

Therefore, it is sufficient to prove that the second term in the right-hand side of (A17) is compact. Actually if so, one can obtain the desired result,
\[ \text{Ind}_{E} = \text{Ind} (\mathcal{P}\mathcal{H}_+\mathcal{P} + 1 - \mathcal{P}) = \text{Ind} (\mathcal{P}\mathcal{U}_+\mathcal{P} + 1 - \mathcal{P}) = \text{Ind}_{B}, \] (A24)
from (A17), (A22) and (A23).

Using \( \mathcal{U} = 1 - 2\mathcal{P}_- \) and the expression (A13) of the projection \( \mathcal{P}_- \), we have
\[ (1 - \mathcal{P})\mathcal{U}\mathcal{P} = (1 - \mathcal{P})(1 - 2\mathcal{P}_-)\mathcal{P} = -2 \times \frac{1}{2\pi i} \int dz \frac{1}{z - H}\mathcal{P}. \] (A25)
From the assumption that the resolvent \((z - H)^{-1}\) exponentially decays with distance at the Fermi level \( E = 0 \), this right-hand side of (A25) is compact. Thus, the second term in the right-hand side of (A17) is compact because \( |H| \) is bounded.

2. D class

In the following two subsections, we treat the classes which show a nontrivial \( \mathbb{Z}_2 \) index. For D class, the Hamiltonian \( H \) has only a particle-hole symmetry. Namely, for an anti-linear transformation \( \Xi \) and for any wavefunction \( \varphi \), the following relation holds:
\[ \Xi H \varphi = -H \Xi \varphi. \] (A26)
Similarly to the preceding case, we write \( \mathcal{P}_\pm \) for the spectral projection onto the positive and negative energies of the Hamiltonian \( H \), respectively. We also write \( \mathcal{U} := \mathcal{P}_+ - \mathcal{P}_- \) for the flattened Hamiltonian. Clearly, one has
\[ \Xi \mathcal{U} \varphi = -\mathcal{U} \Xi \varphi \] (A27)
for any wavefunction \( \varphi \). In the present case, we assume that the Fermi level \( E = 0 \) lies in a nonvanishing spectral gap of the Hamiltonian \( H \). For the case of the mobility gap, our approach below does not work well. This is left for future studies.

The edge Hamiltonian \( H_E \) is defined by \( H_E := \mathcal{P}H\mathcal{P} \), where \( \mathcal{P} \) is the restriction of the whole infinite chain to the half infinite chain. We also assume
\[ \Xi \mathcal{P} \varphi = \mathcal{P} \Xi \varphi \] (A28)
for any wavefunction \( \varphi \). Namely, the particle-hole transformation \( \Xi \) acts on only the internal degree of freedom at each site.

In this class, the bulk \( \mathbb{Z}_2 \) index is defined by [44]
\[ \text{Ind}_{B}^{(2)} := \dim \ker (\mathcal{P}\mathcal{U}\mathcal{P} + 1 - \mathcal{P}) \mod 2. \] (A29)
and the edge \( \mathbb{Z}_2 \) index is defined by
\[ \text{Ind}_{E}^{(2)} := \dim \ker (H_E) \mod 2. \] (A30)
Clearly, this is equal to the even-oddness of the number of the edge zero modes.

Let us give a proof of the equality of the bulk and edge indices. To begin with, we note that
\[ H = \mathcal{P}H\mathcal{P} + \mathcal{P}H(1 - \mathcal{P}) + (1 - \mathcal{P})H\mathcal{P} + (1 - \mathcal{P})H(1 - \mathcal{P}). \] (A31)
Since the range of the hopping amplitudes of the Hamiltonian \( H \) is finite, the second and third terms in the right-hand side are compact operators. Therefore, the essential spectrum of \( H \) is equal to the essential spectrum of \( \mathcal{P}H\mathcal{P} + (1 - \mathcal{P})H(1 - \mathcal{P}) \). (For the stability of an essential spectrum under a compact perturbation, see, e.g., Ref. 48.) This implies that the spectrum of the edge Hamiltonian \( H_E = \mathcal{P}H\mathcal{P} \) which is restricted to the region of the spectral gap of \( H \) is only a subset of the discrete spectrum of \( H_E \).

The edge Hamiltonian \( H_E \) can be written as
\[ H_E = \mathcal{P}H\mathcal{P} = \mathcal{P}H|\mathcal{P}\mathcal{U}\mathcal{P} + \mathcal{P}H|\mathcal{P}H\mathcal{P} + \mathcal{P}H(1 - \mathcal{P})\mathcal{U}\mathcal{P}. \] (A32)
From the assumption of the spectral gap of the Hamiltonian \( H \), in the same way as in the preceding case, one can prove that the second term in the right-hand side of (A32) is a compact operator. We introduce a Hamiltonian,
\[ H_E(g) := \mathcal{P}H|\mathcal{P}\mathcal{U}\mathcal{P} + g\mathcal{P}H|\mathcal{P}H(1 - \mathcal{P})\mathcal{U}\mathcal{P}, \] (A33)
with the parameter \( g \in [0, 1] \). Clearly, \( H_E(1) = H_E \). Let \( \varphi \) be an eigenvector of \( H_E(g) \) with eigenvalue \( \lambda \neq 0 \), i.e., \( H_E(g) \varphi = \lambda \varphi \). Then, one has
\[ H_E(g) \Xi \varphi = -\lambda \Xi \varphi. \] (A34)
Thus, \( \lambda \) and \( -\lambda \) come in pairs of eigenvalues of \( H_E(g) \). On the other hand, the discrete spectrum of \( H_E(g) \) is continuous with respect to the compact perturbation in the spectral gap region. From these observations, we conclude that the even-oddness of the number of the zero modes of \( H_E(g) \) does not depend on the parameter \( g \), i.e.,
\[ \dim \ker (H_E) = \dim \ker (H_E(1)) = \dim \ker (H_E(0)) \mod 2. \] (A35)
The right-hand side can be written as
\[ \dim \ker (H_E(0)) = \dim \ker (\mathcal{P}H(\mathcal{P}\mathcal{U}\mathcal{P} + 1 - \mathcal{P})) = \dim \ker (\mathcal{P}\mathcal{U}\mathcal{P} + 1 - \mathcal{P}), \] (A36)
where we have used \(|H| > 0\) which can be derived from the assumption of the spectral gap at the Fermi level \(E = 0\). These imply the bulk-edge correspondence, \(\text{Ind}_E^{(2)} = \text{Ind}_B^{(2)}\), by the definitions.

3. DIII class

In the final case, the Hamiltonian \(H\) has three symmetries, time-reversal, particle-hole and chiral symmetries whose transformations are, respectively, denoted by \(\Theta\), \(\Xi\) and \(S\). Then, the bulk Hamiltonian \(H\) is transformed as

\[
\Theta H \varphi = H \Theta \varphi, \quad \Xi H \varphi = -H \Xi \varphi \quad \text{and} \quad SH \varphi = -HS \varphi
\]

for any wavefunction \(\varphi\). The two anti-linear transformations, \(\Theta\) and \(\Xi\), satisfy

\[
\Theta^2 \varphi = -\varphi \quad \text{and} \quad \Xi^2 \varphi = \varphi.
\]

(A37)

Further, the relation, \(\Xi = S \Theta\), holds. We assume that the Fermi level \(E = 0\) lies in a nonvanishing spectral gap of the Hamiltonian \(H\).

Similarly to the previous two cases, we define the edge Hamiltonian by \(H_E := PHP\) with the restriction \(P\) of the whole infinite chain to the half infinite chain. We assume that each of the three transformations, \(\Theta\), \(\Xi\) and \(S\), commutes with the restriction \(P\). Since the Hamiltonian \(H\) has the chiral symmetry, the edge Hamiltonian \(H_E\) is decomposed into two parts,

\[
H_E = PH_+P + PH_-P
\]

(A39)

in the same way as in the first case. Therefore, there are two types of zero mode which are also the eigenvectors of the chiral operator \(S\) with eigenvalue \(+1\) and those with eigenvalue \(-1\).

Let \(\varphi\) be a zero edge mode, i.e., \(H_E \varphi = 0\). Then, from the time-reversal symmetry of the Hamiltonian \(H\) and the assumption that the time-reversal transformation \(\Theta\) commutes with \(P\), \(\Theta \varphi\) is also a zero mode. These two states form the Kramers doublet because of the odd time-reversal symmetry \(\Theta^2 = -1\). Namely, the two states satisfy \(\langle \varphi | \Theta \varphi \rangle = 0\). In addition to \(H_E \varphi = 0\), let \(\varphi\) be an eigenvector of the chiral operator \(S\) with eigenvalue \(+1\), i.e., \(S \varphi = \varphi\). Then, one has \(S \Theta \varphi = -\Theta \varphi\). In order to prove this statement, we note that

\[
S \Theta S \Theta \psi = \psi
\]

(A40)

for any wavefunction \(\psi\). This can be obtained from \(\Xi = S \Theta\) and \(\Xi^2 = +1\). Further, by using \(S^2 = 1\) and \(\Theta^2 = -1\), one has

\[
S \Theta \psi = -\Theta S \psi.
\]

(A41)

This yields \(S \Theta \varphi = -\Theta \varphi\) for the wavefunction \(\varphi\) satisfying \(S \varphi = \varphi\). Thus, the two types of the zero modes have the same degeneracy. This implies that the degeneracy of the edge zero modes is always even. Relying on this fact, we define the edge \(\mathbb{Z}_2\) index by

\[
\text{Ind}_E^{(2)} := \frac{1}{2} \dim \ker (H_E) = \frac{1}{2} \dim \ker (PH_+P + PH_-P) \mod 2.
\]

(A42)

In the following, we will use the same notations, \(P_{\pm}\), \(U_1\), and \(U_k\), as in the first case because the Hamiltonian \(H\) has the chiral symmetry in the present case. The bulk \(\mathbb{Z}_2\) index is defined by

\[
\text{Ind}_B^{(2)} := \dim \ker (PH_+P + 1 - P) \mod 2. \quad (A43)
\]

By using the polar decomposition \(H = |H|U\), the edge Hamiltonian \(H_E\) can be written as

\[
H_E = PH|U|P = PH|U|P + PH|1 - P|U|P. \quad (A44)
\]

We again introduce

\[
H_E(g) := |P|H|U|P + g|H|P|U|P \mod 2 \quad (A45)
\]

with the parameter \(g \in [0, 1]\). Clearly, one has \(H_E = H_E(1)\). Note that

\[
SH_E(g) \varphi = -H_E(g)S \varphi
\]

(A46)

and

\[
\Xi H_E(g) \varphi = -H_E(g) \Xi \varphi
\]

(A47)

for any wavefunction \(\varphi\). These imply that, if \(\varphi\) is an energy eigenvector of the edge Hamiltonian \(H_E\) with eigenvalue \(\lambda\), \(S \varphi\) and \(\Xi \varphi\) are also an energy eigenvector of \(H_E\) with eigenvalue \(-\lambda\). Further, we have

\[
\langle S \varphi | \Xi \varphi \rangle = \langle S \varphi | S \Theta \varphi \rangle
\]

\[
= \langle \varphi | \Theta \varphi \rangle = 0,
\]

(A48)

where we have used \(\Xi = S \Theta\), \(S^* S = 1\) and \(\Theta^2 = -1\). Thus, \(\lambda\) and \(-\lambda\) come in pairs of the eigenvalues of \(H_E(g)\) with opposite sign, and both of them have even degeneracy.

Combining these observations about the discrete spectrum of \(H_E(g)\) with the fact that the second term in the right-hand side of (A45) is compact, we have

\[
\frac{1}{2} \dim \ker (H_E) = \frac{1}{2} \dim \ker (H_E(1))
\]

\[
= \frac{1}{2} \dim \ker (H_E(0)) \mod 2. \quad (A49)
\]

On the other hand, we have
where we have used $|H| > 0$ that is obtained from the assumption of the spectral gap of the Hamiltonian $H$. Therefore, we obtain

$$\dim \ker (H_E(0)) = \dim \ker (\mathcal{P} H \mathcal{P} \mathcal{U} \mathcal{P} + 1 - \mathcal{P})$$

$$= 2 \dim \ker (\mathcal{P} \mathcal{U}_+ \mathcal{P} + 1 - \mathcal{P})_{\mathcal{H}_+},$$

(A51)

**Appendix B: Majorana edge zero modes in bond-disordered systems**

In this Appendix, we explain how to construct edge zero modes of the disordered Hamiltonian of Eq. (56).

First, we rewrite the Hamiltonian in terms of the Majorana fermion, in exactly the same way as we have discussed in Sec. II. Then, setting $\langle d_i d_j \rangle = i$ for every $\langle i, j \rangle \in \mathcal{B}_z$, we obtain the Hamiltonian of the free Majorana fermion as

$$H = \sum_{\ell=1}^{L_x} \sum_{m=1}^{L_y} J_x [(2\ell - 1, m), (2\ell, m)] c_{(2\ell - 1, m)} \bar{c}_{(2\ell, m)}$$

$$+ \sum_{\ell=1}^{L_x} \sum_{m=1}^{L_y} J_y [(2\ell, m), (2\ell + 1, m)] c_{(2\ell + 1, m)} \bar{c}_{(2\ell, m)}$$

$$+ \sum_{\ell=1}^{L_x} \sum_{m=1}^{L_y} J_z [(2\ell, m), (2\ell - 1, m + 1)] c_{(2\ell - 1, m + 1)} \bar{c}_{(2\ell, m)}.$$  

(B1)

For this Hamiltonian, we construct a set of zero energy modes which are localized near the left edge. In the following, we assume that the length $L_x$ of the cylinder is large enough, so that the finite-size corrections about $L_x$ are exponentially small in the length $L_x$ and can be neglected.

Consider an operator,

$$\gamma_n = \sum_{\ell=1}^{L_x} \sum_{m=1}^{L_y} U_n(\ell, m) c_{(2\ell - 1, m)},$$

(B2)

where $U_n(\ell, m)$ are real coefficients. This has the same form as in Eq. (35). We determine the coefficients $U_n(\ell, m)$ so that the operator $\gamma_n$ satisfies $[H, \gamma_n] = 0$. Then, the mode $\gamma_n$ satisfies the zero energy condition.
The normalization condition is given by
\[ 1 = \gamma_n^2 = \sum_{\ell=1}^{L_x} \sum_{m=1}^{L_y} |U_n(\ell, m)|^2. \] (B3)

By computing the commutation relation \([H, \gamma_n] = 0\), one obtains
\[ J_y[(2\ell, m), (2\ell + 1, m)]U_n(\ell + 1, m) = J_x[(2\ell - 1, m), (2\ell, m)]U_n(\ell, m) \]
\[ - J_z[(2\ell, m), (2\ell - 1, m + 1)]U_n(\ell, m + 1). \] (B4) (B5)

This implies that the coefficient \(U_n(\ell + 1, m)\) is determined by the two coefficients, \(U_n(\ell, m)\) and \(U_n(\ell, m + 1)\), for a nonvanishing \(J_y[(2\ell, m), (2\ell + 1, m)]\). Therefore, when initial coefficients, \(U_n(1, m)\), for \(m = 1, 2, \ldots, L_y\), are given, all the rest of the coefficients can be determined iteratively. In particular, when the exchange integrals satisfy
\[ |J_x[(2\ell - 1, m), (2\ell, m)]| + |J_z[(2\ell, m), (2\ell - 1, m + 1)]| \leq \kappa |J_y[(2\ell, m), (2\ell + 1, m)]| \] (B6)

with \(\kappa \in (0, 1)\) for all \(\ell, m\), the coefficients, \(U_n(\ell, m)\), decay exponentially in \(\ell\).

For the initial amplitudes, we choose
\[ U_n(1, m) = \delta_{n,m}U_n(1, n) \] (B7)
with a constant \(U_n(1, n) \neq 0\), which is determined by the normalization condition. Then, clearly, one obtains the independent \(L_y\) zero modes, \(\gamma_n\), \((n = 1, \ldots, L_y)\). We remark, however, that \(\gamma_j\)'s are not orthogonal to each other in general, i.e., \(\{\gamma_n, \gamma_{n'}\} \neq 2\delta_{n,n'}\). The orthogonal basis can be obtained by taking the linear combination of \(\gamma_n\) properly. In Fig. 6, the yellow shaded region, which is triangular shaped, shows the area where the amplitude \(U_n(\ell, m)\) may not be vanishing at each black circle site. All the amplitudes at the white circle sites are vanishing.

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