Sublattice-sensitive Majorana Modes

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For two- and three-dimensional topological insulators whose unit cells consist of multiple sublattices, the boundary terminating at which type of sublattice can affect the time-reversal invariant momentum at which the Dirac points of helical boundary states are located. Through a general theory and a representative model, we reveal that this interesting property allows the realization of Majorana modes at sublattice domain walls forming on the boundary when the boundary Dirac points of the topological insulator are gapped by an unconventional superconductor in proximity. Intriguingly, we find that the sensitive sublattice-dependence of the Majorana modes allows their positions to be precisely manipulated by locally controlling the terminating sublattices or boundary potential. Our work reveals that the common sublattice degrees of freedom in materials open a new route to realize and manipulate Majorana modes.

As a class of topological excitations, Majorana modes in topological superconductors (TSCs) have attracted tremendous research enthusiasm since a connection to fault-tolerant quantum computation was built [1,2]. On the road to the final application in quantum computation, it is widely believed that a milestone will be the implementation of braiding Majorana zero modes (MZMs) [3], a type of bound-state Majorana modes. Historically, as MZMs was initially revealed to appear in the vortex cores of two dimensional chiral p-wave superconductors in the topological regime [4], the initial scenario for braiding MZMs is based on the natural idea of moving and exchanging vortices [5]. Later, theorists showed that the braiding process can also be carried out in networks of one-dimensional TSC wires [6,7]. Despite being viewed as two most promising routes, an experimental realization of either one of them remains elusive till date. On one side, although steady and remarkable progress has been witnessed in the pursuit of MZMs in platforms ranging from semiconductor nanowires [8-18] and magnetic atom chains [19-21] to superconducting topological insulators [22-24] and iron-based superconductors [25,27], a decisive confirmation of MZMs in experiments has not been achieved. On the other hand, both scenarios require some levels of controllability on the positions of MZMs, however, manipulating vortex-core or wire-end MZMs in a highly controllable way itself is also rather challenging in experiments.

In the past few years, the birth of the concept named higher-order TSCs provides new perspectives for both the implementation and manipulation of both MZMs and other propagating Majorana modes [28-82]. A unique characteristic of higher-order TSCs is that the concomitant Majorana modes have a codimension \( d_c \) larger than one and their locations in real space depend on the boundary geometry, which is fundamentally distinct to conventional TSCs (also dubbed first-order TSCs) protected by internal symmetries only [83], where the Majorana modes have \( d_c = 1 \) and their locations do not rely on the boundary geometry as they appear everywhere on the whole boundary. Because of the freedom on the boundary, the positions of Majorana modes in a higher-order TSC are in principle allowed to move if the Majorana modes are not pinned by any crystalline symmetry [81-84]. Indeed, previous works have shown that the positions of MZMs in two-dimensional second-order TSCs can be tuned by rotating the orientation of magnetic field [85,86,84], or changing the boundary potential via electrical gating [62,63], accordingly opening new routes to manipulate and braid MZMs [85,87]. In this work, we reveal that the sublattice degrees of freedom commonly appearing in materials admit a new intriguing scheme for the realization and manipulation of Majorana modes with \( d_c = 2 \). Remarkably, this scheme can be applied to systems both with and without time-reversal symmetry (TRS), and allows the positions of Majorana modes to be precisely manipulated.

As putting first-order topological insulators in proximity to unconventional superconductors can provide a natural realization of second-order TSCs [56,58], throughout this work we focus on this class of platforms to illustrate our theory. Accordingly, the physics can be roughly described as follows. For a \( d \)-dimensional first-order topological insulator with \( d > 1 \), while the appearance of helical states does not depend on the terminating sublattice type on the boundary [88,89], a fact, interesting but having attracted little attention, is that the terminating sublattice type can affect the time-reversal invariant momentum (TRIM) at which the Dirac points of helical boundary states are located. On the other hand, it is known that the boundary Dirac points of a topological insulator can be gapped by the Dirac mass induced by the superconductor in proximity [90,91]. Notably, if the superconducting pairing is momentum-dependent, both the magnitude and sign of the superconductivity-induced Dirac mass depend on the location of the boundary Dirac point. This indicates that the terminating sublattice type can directly affect the formation as well as the locations of domain walls binding Majorana modes. Below we first formulate the general theory from a boundary perspective, and then consider a two-dimensional topological insulator with honeycomb lattice and proximity-induced extended s-wave superconductivity to demonstrate the physics.

General theory from a boundary perspective.— Within
the mean-field framework, a superconducting system can be described by a corresponding Bogoliubov de-Gennes (BdG) Hamiltonian of the form $H = \frac{1}{2} \sum_k \Psi_k^\dagger \left[ \mathcal{H}_N(k) + \mathcal{H}_{SC}(k) \right] \Psi_k$, where $\Psi_k$ denotes the normal state, and $\mathcal{H}_{SC}$ describes the superconducting pairing. When $\mathcal{H}_N$ describes a first-order topological insulator with $d > 1$, one knows that helical states will appear on the boundary and form $\Gamma_{\nu}$ for $\nu \in \{\nu_1, \nu_2\}$, where $d > 1$.

The effect of the superconducting pairing to the helical states can be determined by projecting $\mathcal{H}_{SC}$ onto the subspace spanned by the orthogonal wave functions of helical boundary states. In general, if one only considers the leading-order contribution, what the superconducting pairing induces is a constant Dirac mass term to gap out the Dirac point. Accordingly, the low-energy physics on the boundary is described by a massive Dirac Hamiltonian of the form

$$\mathcal{H}_{\nu}(q) = \sum_{i=1}^{d-1} v_i q_i \gamma_i + m_{\nu} \gamma_d,$$

where $\Gamma_{\nu}$ denotes the TRIM at which the boundary Dirac point is located, $q$ is the momentum measured from $\Gamma_{\nu}$, and $\gamma_i$ matrices satisfy the Clifford algebra, i.e., $\{\gamma_i, \gamma_j\} = 2\delta_{ij}$. The effect from the superconducting pairing to the helical states can be determined by projecting $\mathcal{H}_{SC}$ onto the subspace spanned by the orthogonal wave functions of helical boundary states. In general, if one only considers the leading-order contribution, what the superconducting pairing induces is a constant Dirac mass term to gap out the Dirac point. Accordingly, the low-energy physics on the boundary is described by a massive Dirac Hamiltonian of the form

$$\tilde{\mathcal{H}}_{\nu}(q') = \sum_{i=1}^{d-1} v_i q_i' \gamma_i + m_{\nu} \gamma_d,$$

where $q'$ denotes the momentum measured from $\Gamma'_{\nu}$. While the value of Fermi velocity for the helical states on a given boundary may also change, the sign cannot change as each branch of the helical states must propagate in a fixed direction. However, the superconductivity-induced Dirac mass can change its magnitude as well as the sign if the pairing has a momentum dependence, e.g., extended s-wave pairing, d-wave pairing etc. Without loss of generality, let us now consider a nonuniform boundary consisting of two parts which respectively terminate at two distinct types of sublattices. For the convenience of discussion, we dub the interface separating two distinct types of terminating sublattices as sublattice domain walls. Assuming that the sublattice domain walls only break the translation symmetry of the given boundary in the $x_{d-1}$ direction, the boundary Hamiltonian becomes

$$\mathcal{H}(-i\partial_{x_{d-1}}, q'_1) = -iv_{d-1}(x_{d-1})\gamma_{d-1}\partial_{x_{d-1}} + m(x_{d-1})\gamma_d + \sum_{i=1}^{d-2} v_i q'_i \gamma_i,$$

where $q'_1 = (q'_1, ..., q'_{d-2})$ denotes the momentum parallel to the sublattice domain walls. Notably, if $m_{\nu_{1}}$ and $m_{\nu_{2}}$ have opposite signs, then the Dirac mass $m(x_{d-1})$ will change sign across the sublattice domain walls. In other words, the sublattice domain walls are domain walls of Dirac mass. As a result, Majorana modes with $d_c = 2$ will emerge at the sublattice domain walls according to the Jackiw-Rebbi theory [94], corresponding to the realization of an extrinsic time-reversal invariant second-order TSC. As TRS is conserved, the resulting Majorana modes will be Majorana Kramers pairs (two MZMs related by TRS) in two dimensions [46] and propagating helical Majorana modes in three dimensions [43].

The above general theory can be straightforwardly generalized to systems without TRS. Without loss of generality, let us consider that the TRS is broken by an external magnetic field. As Dirac mass induced by superconductivity and Zeeman field will compete, if $|m_{\nu_{1}}| \neq |m_{\nu_{2}}|$ and the absolute value of the Zeeman-field-induced Dirac mass falls between $|m_{\nu_{1}}|$ and $|m_{\nu_{2}}|$, the Dirac mass of domain walls will be dominated by Zeeman field on one side and by superconductivity on the other side [93]. As a result, the Majorana Kramers pairs and helical Majorana modes will respectively change to single MZMs and chiral Majorana modes, with their locations still bound at the sublattice domain walls [93]. With the established general theory in mind, below we consider a concrete realization to demonstrate the discussed physics.

Kane-Mele model with spin-singlet pairing.— Since two-dimensional honeycomb lattices with just two types of sublattices allow a simple illustration of the essential physics, below we consider the representative Kane-Mele model to describe the topological insulator and further assume a proximity-induced spin-singlet pairing. The full Hamiltonian has the form

$$H = t \sum_{\langle ij \rangle, \alpha} c_{i,\alpha}^\dagger c_{j,\alpha} + i\lambda_0 \sum_{\langle ij \rangle, \alpha, \beta} \nu_{ij} c_{i,\alpha}^\dagger c_{j,\beta} + \mu \sum_{i, \alpha} c_{i,\alpha}^\dagger c_{i,\alpha} + \Delta_0 \sum_{i} c_{i,\uparrow}^\dagger c_{i,\downarrow} + \Delta_{1,ij} c_{i,\uparrow}^\dagger c_{i,\downarrow} + \Delta_{2,ij} c_{i,\uparrow}^\dagger c_{j,\downarrow} + h.c.,$$

where $\langle ij \rangle$ and $\langle \langle ij \rangle \rangle$ refer to nearest-neighbor and next-nearest-neighbor sites. The first line corresponds to the Kane-Mele model which realizes a two-dimensional first-order topological insulator as long as the spin-orbit coupling coefficient $\lambda_0$ is nonzero [95, 96]. $\mu$ is the chemical potential,
\(\Delta_0\), \(\Delta_{1,ij}\) and \(\Delta_{2,ij}\) represent the on-site, nearest-neighbor and next-nearest-neighbor pairings, respectively. To have momentum dependence in the pairing, at least one of \(\Delta_{1,ij}\) and \(\Delta_{2,ij}\) needs to be nonzero. It is worth noting that according to the general theory, there is no constraint on the pairing type (a demonstration of the physics via d-wave pairing is provided in the supplemental material [22]). Without loss of generality, below we assume \(\Delta_{1,ij} = \Delta_1\) and \(\Delta_{2,ij} = \Delta_2\) for simplicity, corresponding to an extended s-wave pairing which preserves all crystalline symmetry of the normal-state Hamiltonian.

By a Fourier transformation to the momentum space and choosing the basis to be \(\Psi_k^\dagger = (\psi_k^\dagger, \psi_{-k})\) with \(\psi_k = (c_{A,k,\uparrow}, c_{B,k,\uparrow}, c_{A,k,\downarrow}, c_{B,k,\downarrow})\), the BdG Hamiltonian reads

\[
\mathcal{H}(k) = t \sum_i \left[ \cos(\mathbf{k} \cdot \mathbf{a}_i) \tau_z s_0 \sigma_x + \sin(\mathbf{k} \cdot \mathbf{a}_i) \tau_z s_0 \sigma_y \right]
+ 2\lambda_{so} \sum_i \sin(\mathbf{k} \cdot \mathbf{b}_i) \tau_0 s_2 \sigma_z - \mu \tau_0 s_0 \sigma_0
- \Delta_1 \sum_i \left[ \cos(\mathbf{k} \cdot \mathbf{a}_i) \tau_y s_y \sigma_x + \sin(\mathbf{k} \cdot \mathbf{a}_i) \tau_y s_y \sigma_y \right]
- [\Delta_0 + 2\Delta_2 \sum_i \cos(\mathbf{k} \cdot \mathbf{b}_i)]\tau_y s_y \sigma_0,
\]

where the Pauli matrices \(\tau_i\), \(s_i\) and \(\sigma_j\) act on the particle-hole, spin (\(\uparrow, \downarrow\)) and sublattice \((A, B)\) degrees of freedom, respectively. The sum runs over \(i = 1, 2, 3\), with the nearest-neighbor vectors \(\mathbf{a}_1 = a(0,1), \mathbf{a}_2 = \frac{2}{3}(\sqrt{3}, -1), \mathbf{a}_3 = \frac{2}{3}(-\sqrt{3}, -1)\), and \(a\) being the lattice constant (below we set \(a = 1\) for notational simplicity). The next-nearest-neighbor vectors \(\mathbf{b}_1 = \mathbf{a}_2 - \mathbf{a}_3, \mathbf{b}_2 = \mathbf{a}_3 - \mathbf{a}_1\) and \(\mathbf{b}_3 = \mathbf{a}_1 - \mathbf{a}_2\). [27].

The Hamiltonian has TRS (the time-reversal operator \(T = \tau_0 s_0 \sigma_0 K\) with \(K\) the complex conjugate operator), particle-hole symmetry \((P = \tau_0 s_0 \sigma_0 K)\), and inversion symmetry \((I = \tau_0 s_0 \sigma_0)\). Because the coexistence of TRS and inversion symmetry enforces Kramers degeneracy to the bulk bands, the first-order topology of the BdG Hamiltonian will always be trivial for the concerned spin-singlet pairing [70, 75, 88]. In previous works, it has been shown that a topological insulator with square lattice in proximity to an extended s-wave superconductor can realize a second-order TSC with Majorana Kramers pairs localized at the corners of a square sample [66]. Notably, therein the topological criterion requires either the hopping or the domain walls to have crystalline anisotropy, because otherwise domain walls of Dirac mass cannot form on the boundary due to symmetry constraint. However, as we will show below, even though both the hopping and pairing are considered to be isotropic in Eq. (7), here domain walls of Dirac mass can still form on the boundary due to the sublattice degrees of freedom.

For the honeycomb lattice, there are two kinds of simple boundaries whose outermost sublattices only contain one type, which are known as zigzag and beard boundaries (see Figs.1(a)(b)). Let us first investigate the influence of the change of terminating sublattice type on a given boundary to the helical edge states of the normal state. To be specific, we consider a cylindrical geometry with periodic boundary condition in the \(x\) direction and open boundary condition in the \(y\) direction. When the upper edge terminates at type-B sublattices and the lower edge terminates at type-A sublattices (see Fig.1(a)), one finds that the boundary Dirac points for both upper and lower edges are located at \(k_x = \pi/\sqrt{3}\), as shown in Fig.1(c). By only changing the terminating sublattice type on the upper edge, one finds that one boundary Dirac point is immediately shifted from \(k_x = \pi/\sqrt{3}\) to \(k_x = 0\), as shown in Figs.1(b)(d). Since nothing changes in the bulk as well as on the lower edge, the shifted Dirac point apparently corresponds to the upper edge, indicating the sensitive sublattice-dependence of boundary Dirac points.

Taking into account the superconductivity, numerical results show that the on-site pairing, nearest-neighbor pairing and next-nearest-neighbor pairing have rather different effects to the helical edge states, as shown in Fig.2. The on-site pairing, as expected, will induce a Dirac mass to gap out the Dirac points, irrespective of whether the edge is zigzag-type or beard-type, as shown in Fig.2(a). In sharp contrast, Fig.2(b) shows that the boundary Dirac points are intact to the nearest-neighbor pairing. Last, the next-nearest-neighbor pairing turns out to open a gap for the Dirac point of the zigzag boundary but not for that of the beard boundary, as shown in Fig.2(c). These results indicate when both \(\Delta_0\) and \(\Delta_2\) are finite, the gaps opened for the Dirac points at \(k_x = 0\) and \(k_x = \pi/\sqrt{3}\) can be different, as shown in Fig.2(d).

As the effect of the nearest-neighbor pairing to the helical edge states is negligible, below we set \(\Delta_1 = 0\) for simplicity. To obtain the topological criterion for the emergence of domain walls binding Majorana modes, we follow the general theory and derive the low-energy boundary Hamiltonians for both zigzag and beard edges [22]. Focusing on the upper \(y\)-normal boundary and considering the case with \(\mu = 0\)
where \( v_{\text{at type-B sublattices}} \) is the boundary Hamiltonian for the zigzag-type edge (terminating at type-A sublattices) is

\[
H_{u,\text{beard}}(q_x) = v q_x \tau_0 s_z - \Delta_0 \tau_y s_y, \tag{8}
\]

where \( v = 3 \sqrt{3} \lambda_{so} \) and \( q_x \) is measured from \( k_x = 0 \), and the boundary Hamiltonian for the zigzag-type edge (terminating at type-B sublattices) is

\[
H_{u,\text{zigzag}}(q'_x) = v' q'_x \tau_0 s_z + (2\Delta_2 - \Delta_0) \tau_y s_y, \tag{9}
\]

where \( v' \approx 6 \sqrt{3} \lambda_{so} / t \ll 1 \), and \( q'_x \) is measured from \( k_x = \pi / \sqrt{3} \). It is easy to find that the Dirac masses in the two Hamiltonians will take opposite signs if \( |\Delta_1| > |\Delta_0| / 2 > 0 \). This is the topological criterion for sublattice domain walls to host Majorana Kramers pairs at \( \mu = 0 \). Due to the robustness of topology, this topological criterion will hold as long as \( \mu \) is lower than the critical value at which the boundary energy gap gets closed.

To validate the established topological criterion, we still consider a cylindrical geometry with periodic boundary condition in the \( x \) direction and just let the upper edge be nonuniform, with one part terminating at B-type sublattices (zigzag) and the other part terminating at A-type sublattices (beard). Accordingly, there are two sublattice domain walls on the upper edge, while the lower edge keeps uniform. As shown in Fig. 3 when the topological criterion is fulfilled, a diagonalization of the Hamiltonian shows the existence of four MZMs, corresponding to two Majorana Kramers pairs. As expected, the wave functions of Majorana Kramers pairs are strongly localized around the sublattice domain walls. In addition, by a comparison of Figs. 3(a) and (b), it is readily seen that the positions of Majorana Kramers pairs directly follow the change of the positions of sublattice domain walls, indicating that the positions of Majorana Kramers pairs can be tuned site-by-site by a precise control of the terminating sublattices. Remarkably, even when the positions of sublattice domain walls are fixed, we find that the same goal can also be achieved by electrically tuning the local boundary potential.

**Discussion and conclusion.**—While our theory is exemplified in terms of the two-dimensional honeycomb lattice, its generality admits a wide application as sublattice degrees of freedom are rather common in materials, e.g., the class of materials with kagome or Lieb lattice consist of three types of sublattices. As a new scheme for the implementation of extrinsic second-order TSCs and Majorana modes, one remarkable merit is that the sensitive sublattice-dependence allows the positions of Majorana modes to be manipulated at an atomically precise level. Therefore, our work opens a promising avenue for achieving the manipulation and braiding of Majorana modes.

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I. THE DERIVATION OF LOW-ENERGY BOUNDARY HAMILTONIANS FOR BEARD AND ZIGZAG EDGES

To derive the low-energy boundary Hamiltonian, we write down the bulk Bogoliubov-de Gennes (BdG) Hamiltonian in an explicit form, which reads

$$H_{\text{BdG}}(k) = t(2\cos \frac{\sqrt{3}k_x}{2} \cos \frac{k_y}{2} + \cos k_y)\tau_z s_0 \sigma_x - t(2\cos \frac{\sqrt{3}k_x}{2} \sin \frac{k_y}{2} - \sin k_y)\tau_z \sigma_y$$

$$+ 2\lambda_{so}(\sin \sqrt{3}k_x - 2\sin \frac{\sqrt{3}k_x}{2} \cos \frac{3k_y}{2})\tau_0 s_z \sigma_z - \mu \tau_z s_0 \sigma_0$$

$$- \Delta_1(2\cos \frac{\sqrt{3}k_x}{2} \cos \frac{k_y}{2} + \cos k_y)\tau_y s_y \sigma_x + \Delta_1(2\cos \frac{\sqrt{3}k_x}{2} \sin \frac{k_y}{2} - \sin k_y)\tau_y s_y \sigma_y$$

$$- [\Delta_0 + 2\Delta_2(\cos \sqrt{3}k_x + 2\cos \frac{3k_y}{2})\tau_y s_y \sigma_0].$$ (S1)

For notational simplicity, we have set the lattice constant to unity. For the convenience of discussion, throughout this work, $t$ and $\lambda_{so}$ will be assumed to be positive. As we have shown numerically that the nearest-neighbor pairing has a negligible effect to the helical edge states, below we also set $\Delta_1 = 0$ for simplicity.

According to numerical results, we know that for a cylindrical geometry with periodic boundary condition in the $x$ direction and open boundary condition in the $y$ direction, the boundary Dirac point, which corresponds to the crossing point of the energy spectrum of the normal-state helical edge states, is located at $k_x = 0$ ($k_x = \pi/\sqrt{3}$) for a beard (zigzag) edge. Below let us focus on the upper $y$-normal boundary and derive the corresponding low-energy boundary Hamiltonians for both beard and zigzag edges.

A. Low-energy boundary Hamiltonian for the beard edge

When the upper boundary is a beard edge, the terminating sublattices are type A. As numerical calculations reveal that the boundary Dirac point for such an edge will appear at $k_x = 0$, in order to derive the low-energy boundary Hamiltonian, we perform an expansion of the bulk Hamiltonian around $k_x = 0$ up to the linear order in momentum. Accordingly, the Hamiltonian becomes

$$H_{\text{BdG}}(q_x, k_y) = t(2\cos \frac{k_y}{2} + \cos k_y)\tau_z s_0 \sigma_x - t(2\sin \frac{k_y}{2} - \sin k_y)\tau_z \sigma_y$$

$$+ 2\sqrt{3}\lambda_{so}q_x(1 - \cos \frac{3k_y}{2})\tau_0 s_z \sigma_z - \mu \tau_z s_0 \sigma_0$$

$$- [\Delta_0 + 2\Delta_2(1 + 2\cos \frac{3k_y}{2})\tau_y s_y \sigma_0].$$ (S2)

where $q_x$ denotes a small momentum measured from $k_x = 0$. Next, we decompose the Hamiltonian into two parts, $H_{\text{BdG}} = H_1 + H_2$, with

$$H_1(q_x, k_y) = t(2\cos \frac{k_y}{2} + \cos k_y)\tau_z s_0 \sigma_x - t(2\sin \frac{k_y}{2} - \sin k_y)\tau_z s_0 \sigma_y,$$

$$H_2(q_x, k_y) = 2\sqrt{3}\lambda_{so}q_x(1 - \cos \frac{3k_y}{2})\tau_0 s_z \sigma_z - \mu \tau_z s_0 \sigma_0 - [\Delta_0 + 2\Delta_2(1 + 2\cos \frac{3k_y}{2})\tau_y s_y \sigma_0].$$ (S3)
For real materials, $\lambda_{so} \ll t$ and $\Delta_{0.2} \ll t$ are naturally satisfied. As we are interested in the regime where $q_z$ is small, the whole $H_2$ can be treated as a perturbation if the chemical potential is also assumed to be close to the neutrality condition.

In the following, let us consider a half-infinity sample with the boundary corresponding to the upper bond edge. In the basis $\Psi_{q_z} = (\psi_{1A,q_z}, \psi_{1B,q_z}, \psi_{2A,q_z}, \psi_{2B,q_z}, ..., \psi_{nA,q_z}, \psi_{nB,q_z}, ...)^T$ with $\psi_{nA,B,q_z} = (\psi_{nA(B),q_z}, \psi_{nA(B),q_z}^\dagger)$, the Hamiltonian in the matrix form reads

$$H_1 = \begin{pmatrix}
0 & t_{\tau s} & 0 & 0 & 0 & \cdots \\
t_{\tau s} & 0 & 2t_{\tau s} & 0 & 0 & \cdots \\
0 & 2t_{\tau s} & 0 & t_{\tau s} & 0 & \cdots \\
0 & 0 & t_{\tau s} & 0 & 2t_{\tau s} & 0 & \cdots \\
0 & 0 & 0 & t_{\tau s} & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}.$$  \hspace{1cm} \text{(S4)}

To see that this Hamiltonian has solutions for zero-energy bound states, we solve the eigenvalue equation $H_1|\Psi_\alpha\rangle = 0$. Concretely, as $\tau_s$ and $s_z$ both commute with $H_1$, the eigenvector $|\Psi_\alpha\rangle$ can be assigned with the form

$$|\Psi_{\tau s}\rangle = |\tau_s = \tau\rangle \otimes |s_z = s\rangle \otimes (\psi_{1A}, \psi_{1B}, \psi_{2A}, \psi_{2B}, ..., \psi_{nA}, \psi_{nB}, ...)^T,$$  \hspace{1cm} \text{(S5)}

where $\tau = \pm 1$ and $s = \pm 1$ correspond to the two possible eigenvalues of $\tau_z$ and $s_z$, respectively. Taking the expression of $|\Psi_{\tau s}\rangle$ back into the eigenvalue equation $H_1|\Psi_{\tau s}\rangle = 0$, one gets a series of equations with periodic structures, which read

$$t_\tau \psi_{1B} = 0,$$

$$t_\tau \psi_{1A} + 2t_\tau \psi_{2A} = 0,$$

$$2t_\tau \psi_{1B} + t_\tau \psi_{2B} = 0,$$

$$...$$

$$t_\tau \psi_{nA} + 2t_\tau \psi_{(n+1)A} = 0,$$

$$2t_\tau \psi_{nB} + t_\tau \psi_{(n+1)B} = 0,$$

$$...$$

where $t_\tau = t \tau$. According to the periodic structures, one can easily find

$$\psi_{(n+1)A} = -\frac{1}{2} \psi_{nA}, \quad \psi_{nB} = 0.$$  \hspace{1cm} \text{(S7)}

Therefore, the eigenvectors take the form

$$|\Psi_{\tau s}\rangle = |\tau_z = \tau\rangle \otimes |s_z = s\rangle \otimes \mathcal{N}(1, 0, -\frac{1}{2}, 0, ..., (-\frac{1}{2})^{(n-1)}, 0, ...)^T,$$  \hspace{1cm} \text{(S8)}

where the normalization constant $\mathcal{N}$ is determined by the normalization condition $\langle \Psi_{\tau s}|\Psi_{\tau s}\rangle = 1$. Simple algebra calculations give

$$\mathcal{N}^2 \sum_{n=0}^{\infty} \frac{1}{2^{2n}} = \mathcal{N}^2 \left(1 - \frac{1}{4}\right) = \frac{4}{3} \mathcal{N}^2 = 1,$$  \hspace{1cm} \text{(S9)}

indicating $\mathcal{N} = \sqrt[3]{\frac{4}{3}}$. As $\psi_{nA}$ decays in a power law with the increase of $n$, the existence of four such eigenvectors indicates the existence of four zero-energy bound states. It is worth noting that the topological insulator has one pair of helical states on a given edge, but the introduce of particle-hole degrees of freedom doubles the number of helical states. Next, we project $H_2$ onto the basis spanned by the four zero-energy eigenvectors. To proceed, we write down the matrix form for each term in $H_2$.

Let us first focus on the term $H_{2,1} = 2\sqrt{3}\lambda_{so}q_z(1 - \cos \frac{k_y}{2})\tau_0 s_z \sigma_z$. In the basis $\Psi_{q_z} = (\psi_{1A,q_z}, \psi_{1B,q_z}, \psi_{2A,q_z}, \psi_{2B,q_z}, ..., \psi_{nA,q_z}, \psi_{nB,q_z}, ...)^T$, its matrix form is

$$H_{2,1} = \tau_0 \otimes s_z \otimes \begin{pmatrix}
2\sqrt{3}\lambda_{so}q_z & 0 & -\sqrt{3}\lambda_{so}q_z & 0 & 0 & 0 & \cdots \\
0 & -2\sqrt{3}\lambda_{so}q_z & 0 & \sqrt{3}\lambda_{so}q_z & 0 & 0 & \cdots \\
-\sqrt{3}\lambda_{so}q_z & 0 & 2\sqrt{3}\lambda_{so}q_z & 0 & -\sqrt{3}\lambda_{so}q_z & 0 & \cdots \\
0 & \sqrt{3}\lambda_{so}q_z & 0 & -2\sqrt{3}\lambda_{so}q_z & 0 & \sqrt{3}\lambda_{so}q_z & \cdots \\
0 & 0 & -\sqrt{3}\lambda_{so}q_z & 0 & 2\sqrt{3}\lambda_{so}q_z & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}.$$  \hspace{1cm} \text{(S10)}
Then the contribution from $\mathcal{H}_{2,1}$ to the boundary Hamiltonian is

\[
(\mathcal{H}_{\text{beard},1})_{\tau_s,\tau_{s'}} = \langle \Psi_{\tau_s} | \mathcal{H}_{2,1} | \Psi_{\tau_{s'}} \rangle \\
= 2\sqrt{3} \lambda_{so,ss} q_x \delta_{\tau_s \tau_{s'}} \delta_{ss'} - \sqrt{3} \lambda_{so,ss} q_x \delta_{\tau_s \tau_{s'}} \delta_{ss'} N^2 \sum_{n=1}^{+\infty} 2\psi_{nA} \psi_{(n+1)A} \\
= 2\sqrt{3} \lambda_{so,ss} q_x \delta_{\tau_s \tau_{s'}} \delta_{ss'} + \sqrt{3} \lambda_{so,ss} q_x \delta_{\tau_s \tau_{s'}} \delta_{ss'} N^2 \sum_{n=1}^{+\infty} \psi_{nA} \psi_{nA} \\
= 2\sqrt{3} \lambda_{so,ss} q_x \delta_{\tau_s \tau_{s'}} \delta_{ss'} + \sqrt{3} \lambda_{so,ss} q_x \delta_{\tau_s \tau_{s'}} \delta_{ss'} \\
= 3\sqrt{3} \lambda_{so,ss} q_x \delta_{\tau_s \tau_{s'}} \delta_{ss'},
\]

(S11)

where $\lambda_{so,ss} \equiv \lambda_{so}$. In the derivation above, a few facts have been used, including: (1) $\psi_{nA}$ is real; (2) $\psi_{(n+1)A} = -\frac{1}{2} \psi_{nA}$; (3) $N^2 \sum_{n=1}^{+\infty} \psi_{nA}^2 = 1$. Choosing the basis spanning the subspace for boundary Hamiltonian to be $\{|\Psi_1\rangle, |\Psi_{-1}\rangle, |\Psi_{-1}\rangle, |\Psi_{-1}\rangle\}$, $\mathcal{H}_{\text{beard},1}$ can be expressed in terms of the Pauli matrices as

\[
\mathcal{H}_{\text{beard},1} = 3\sqrt{3} \lambda_{so} q_x \tau_0 s_z.
\]

(S12)

For the second term $\mathcal{H}_{2,2} = -\mu \tau_z s_0 \sigma_0$, as it is diagonal in the basis $\Psi_{q_x}$, one can easily find that its contribution to the boundary Hamiltonian is just

\[
\mathcal{H}_{\text{beard},2} = -\mu \tau_z s_0.
\]

(S13)

Now let us analyze the contribution from the pairing term. In the basis $\Psi_{q_x}$, the matrix form of the pairing term is

\[
\mathcal{H}_{2,3} = \begin{pmatrix}
(\Delta_0 + 2\Delta_2)\tau_y s_y & 0 & 2\Delta_2 \tau_y s_y & 0 & \cdots \\
0 & (\Delta_0 + 2\Delta_2)\tau_y s_y & 0 & 2\Delta_2 \tau_y s_y & \cdots \\
2\Delta_2 \tau_y s_y & 0 & (\Delta_0 + 2\Delta_2)\tau_y s_y & 0 & \cdots \\
0 & 2\Delta_2 \tau_y s_y & 0 & (\Delta_0 + 2\Delta_2)\tau_y s_y & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}.
\]

(S14)

Similarly, its contribution to the boundary Hamiltonian is

\[
\langle \Psi_{\tau_s} | \mathcal{H}_{2,3} | \Psi_{\tau_{s'}} \rangle = -\Delta_0 \tau_y s_y
\]

One finds that the contribution from the next-nearest-neighbor pairing will vanish for the beard edge, in agreement with the numerical results shown in Fig.2 of the main text. In terms of the Pauli matrices, its form is just

\[
\mathcal{H}_{\text{beard},3} = -\Delta_0 \tau_y s_y.
\]

(S16)

Taking all contributions together, we reach the final expression of the boundary Hamiltonian for the upper beard edge, which reads

\[
\mathcal{H}_{\text{beard}} = \mathcal{H}_{\text{beard},1} + \mathcal{H}_{\text{beard},2} + \mathcal{H}_{\text{beard},3} = v q_x \tau_0 s_z - \mu \tau_z s_0 - \Delta_0 \tau_y s_y,
\]

(S17)

where $v = 3\sqrt{3} \lambda_{so}$. In the limit $\mu = 0$, the boundary Hamiltonian reduces to the form of Eq.(8) in the main text. We find that the boundary energy gap at $k_x = 0$ predicted by the low-energy boundary Hamiltonian agree perfectly with the numerical results when only the on-site pairing or the next-nearest-neighbor pairing is present. When both the on-site and the next-nearest-neighbor pairings are finite, the boundary energy gap is found to be a little smaller than the predicted value $E_g = 2|\Delta_0|$, but the agreement is still very good at the neighborhood of the boundary Dirac point.
B. Low-energy boundary Hamiltonian for the zigzag edge

When the upper edge changes to terminate at type-B sublattices, so a zigzag edge, numerical results show that the boundary Dirac point is shifted to \( k_x = \pi / \sqrt{3} \). In order to analytically derive the corresponding boundary Hamiltonian, we similarly perform an expansion around \( k_x = \pi / \sqrt{3} \) and keep the momentum up to the linear order. Accordingly, the Hamiltonian becomes

\[
\mathcal{H}_{BDG}(q'_x, k_y) = t(-\sqrt{3}q'_x \cos \frac{k_y}{2} + \cos k_y)\tau_z s_0 \sigma_x + t(\sqrt{3}q'_x \sin \frac{k_y}{2} + \sin k_y)\tau_z s_0 \sigma_y + 2\lambda_{so}(\sqrt{3}q'_x - 2 \cos \frac{3k_y}{2})\tau_0 s_z \sigma_z - \mu \tau_z s_0 \sigma_0 - |\Delta_0 + 2\Delta_2(-1 - \sqrt{3}q'_x \cos \frac{3k_y}{2})|\tau_y s_y \sigma_0,
\]

(S18)

where \( q'_x \) denotes a small momentum measured from \( k_x = \pi / \sqrt{3} \). Similar to the previous case, we decompose the Hamiltonian into two parts, \( \mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 \), with

\[
\mathcal{H}_1(q'_x, k_y) = t \cos k_y \tau_z s_0 \sigma_x + t \sin k_y \tau_z s_0 \sigma_y - 4\lambda_{so} \cos \frac{3k_y}{2} \tau_0 s_z \sigma_z,
\]

\[
\mathcal{H}_2(q'_x, k_y) = -\sqrt{3}tq'_x \cos k_y \tau_z s_0 \sigma_x + \sqrt{3}tq'_x \sin k_y \tau_z s_0 \sigma_y - 2\lambda_{so}q'_x \tau_0 s_z \sigma_z - \mu \tau_z s_0 \sigma_0 - |\Delta_0 + 2\Delta_2(-1 - \sqrt{3}q'_x \cos \frac{3k_y}{2})|\tau_y s_y \sigma_0.
\]

(S19)

As we are interested in the small \( q'_x \) regime, it is also justified to treat the whole \( \mathcal{H}_2 \) as a perturbation.

When the upper edge becomes a zigzag one, the terminating sublattices become type B, so the corresponding basis for a half-infinity system becomes \( \Psi_{q'_x} = (c_{1B, q'_x}, c_{2, A, q'_x}, c_{2, B, q'_x}, c_{3, A, q'_x}, c_{3, B, q'_x}, ... , c_{n, A, q'_x}, c_{n, B, q'_x}, ...)^T \). Then \( \mathcal{H}_1 \) in matrix form reads

\[
\mathcal{H}_1 = \begin{pmatrix}
0 & 0 & 2\lambda_{so}\tau_0 s_z & 0 & 0 & 0 & 0 & \cdots \\
0 & 0 & t\tau_z s_0 & -2\lambda_{so}\tau_0 s_z & 0 & 0 & 0 & \cdots \\
2\lambda_{so}\tau_0 s_z & t\tau_z s_0 & 0 & 0 & 2\lambda_{so}\tau_0 s_z & 0 & 0 & \cdots \\
0 & -2\lambda_{so}\tau_0 s_z & 0 & 0 & t\tau_z s_0 & -2\lambda_{so}\tau_0 s_z & 0 & \cdots \\
0 & 0 & 2\lambda_{so}\tau_0 s_z & t\tau_z s_0 & 0 & 0 & 0 & \cdots \\
0 & 0 & 0 & t\tau_z s_0 & 0 & 0 & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix},
\]

(S20)

As \( \tau_z \) and \( s_z \) also commute with \( \mathcal{H}_1 \), the zero-energy eigenvectors of \( \mathcal{H}_1 \) can also be assigned the form

\[
|\Psi_{s_z}\rangle = |\tau_z = \tau\rangle \otimes |s_z = s\rangle \otimes (\psi_{1B}, \psi_{2A}, \psi_{2B}, \psi_{3A}, \psi_{3B}, ..., \psi_{nA}, \psi_{nB})^T.
\]

(S21)

Accordingly, the eigenvalue equation \( \mathcal{H}_1|\Psi_{s_z}\rangle = 0 \) leads to the following equations with periodic structures,

\[
2\lambda_{so, s}\psi_{2B} = 0,
\]

\[
t\psi_{2B} - 2\lambda_{so, s}\psi_{3A} = 0,
\]

\[
2\lambda_{so, s}\psi_{1B} + t\psi_{2A} + 2\lambda_{so, s}\psi_{3B} = 0,
\]

\[
-2\lambda_{so, s}\psi_{2A} + t\psi_{3B} - 2\lambda_{so, s}\psi_{4A} = 0,
\]

\[
2\lambda_{so, s}\psi_{(n-1)B} + t\psi_{nA} + 2\lambda_{so, s}\psi_{(n+1)B} = 0,
\]

\[
-2\lambda_{so, s}\psi_{nA} + t\psi_{(n+1)B} - 2\lambda_{so, s}\psi_{(n+2)A} = 0,
\]

\[
\vdots
\]

(S22)

It is readily found that the components of eigenvectors have \( \psi_{(2n)B} = \psi_{(2n+1)A} = 0 \). Therefore, we only need to focus on the following equations,

\[
2\lambda_{so, s}\psi_{(2n-1)B} + t\psi_{(2n)A} + 2\lambda_{so, s}\psi_{(2n+1)B} = 0,
\]

\[
-2\lambda_{so, s}\psi_{(2n)A} + t\psi_{(2n+1)B} - 2\lambda_{so, s}\psi_{(2n+2)A} = 0.
\]

(S23)
Consider the trial function
\[
\begin{pmatrix}
\psi_{(2n+1)B} \\
\psi_{(2n+2)A}
\end{pmatrix} = \xi^n \begin{pmatrix}
\psi_1 B \\
\psi_2 A
\end{pmatrix},
\] (S24)
where \(|\xi| < 1\) is required so that the wave function decays in real space and corresponds to a bound state. Accordingly, one finds that the series of equations reduce to two algebra equations, which read
\[
2\lambda_{s_0,s} \psi_{1B} + t_\tau \psi_{2A} + 2\lambda_{s_0,s} \xi \psi_{1B} = 0,
-2\lambda_{s_0,s} \psi_{2A} + t_\tau \xi \psi_{1B} - 2\lambda_{s_0,s} \xi \psi_{2A} = 0.
\] (S25)
By simple algebra, one finds
\[
\psi_{1B} = -\frac{t_\tau}{2\lambda_{s_0,s}(1 + \xi)} \psi_{2A},
\frac{2\lambda_{s_0,s}(1 + \xi)}{t_\tau \xi} = -\frac{t_\tau}{2\lambda_{s_0,s}(1 + \xi)}.
\] (S26)
There are two solutions for \(\xi\),
\[
\xi_\pm = \frac{-(t_\tau^2 + 8\lambda_{s_0,s}^2) \pm \sqrt{t_\tau^2(t_\tau^2 + 16\lambda_{s_0,s}^2)}}{8\lambda_{s_0,s}},
\] (S27)
however, only \(\xi_+\) leads to decaying wave functions, so bound states. Taking \(\xi_+\) back into Eq. (S26), one finds
\[
\psi_{1B} = \frac{4t_\tau \lambda_{s_0,s}}{\lambda_{s_0,s}(t_\tau^2 - \sqrt{t_\tau^2(t_\tau^2 + 16\lambda_{s_0,s}^2)})} \psi_{2A} \equiv \tau_{\tau s} \psi_{2A} = -\tau s |\eta_{\tau s}| \psi_{2A}.
\] (S28)
As \(\tau\) and \(s\) have four possible combinations, there are also four eigenvectors corresponding to four zero-energy bound states. The eigenvectors can also be expressed as
\[
|\Psi_{\tau s}\rangle = |\tau_z = \tau\rangle \otimes |s_z = s\rangle \otimes \mathcal{N}(|\eta_{\tau s}, 1, 0, 0, \xi_+ \eta_{\tau s}, \xi_+, 0, 0, \xi_+^2 \eta_{\tau s}, \xi_+^2, \ldots)\rangle.
\] (S29)
The normalization condition \(|\Psi_{\tau s}\rangle |\Psi_{\tau s}\rangle = 1\) gives
\[
\mathcal{N}^2(1 + \eta_{\tau s}^2) \sum_{n=0}^{\infty} \xi_+^{2n} = \mathcal{N}^2 \frac{(1 + \eta_{\tau s}^2)}{1 - \xi_+^2} = 1,
\] (S30)
which indicates
\[
\mathcal{N} = \sqrt{\frac{1 - \xi_+^2}{1 + \eta_{\tau s}^2}}.
\] (S31)
Let us now analyze the effect of \(\mathcal{H}_2\). For the first two terms in \(\mathcal{H}_2\), \(\mathcal{H}_{2,1+2} = -\sqrt{3}tq_x' \cos \frac{k_y}{2} \tau_z s_0 \sigma_y + \sqrt{3}tq_x' \sin \frac{k_y}{2} \tau_z s_0 \sigma_y\), the corresponding matrix form reads
\[
\mathcal{H}_{2,1+2} = \begin{pmatrix}
0 & -\sqrt{3}tq_x' \tau_z s_0 & 0 & 0 & 0 & 0 & 0 & \cdots \\
-\sqrt{3}tq_x' \tau_z s_0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\
0 & 0 & -\sqrt{3}tq_x' \tau_z s_0 & 0 & 0 & 0 & 0 & \cdots \\
0 & 0 & 0 & -\sqrt{3}tq_x' \tau_z s_0 & 0 & 0 & 0 & \cdots \\
0 & 0 & 0 & 0 & -\sqrt{3}tq_x' \tau_z s_0 & 0 & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}.
\] (S32)
By projecting \(\mathcal{H}_{2,1+2}\) onto \(|\Psi_{\tau s}\rangle\), one finds its contribution to the boundary Hamiltonian, which reads
\[
(\mathcal{H}_{\text{zigzag}})_{\tau s, \tau' s'} = \langle \Psi_{\tau s}^\dagger | \mathcal{H}_{2,1+2} | \Psi_{\tau' s'} \rangle
= -2\sqrt{3}tq_x' \tau \eta_{\tau s} \delta_{\tau \tau'} \delta_{ss'} \mathcal{N}^2 \sum_{n=0}^{\infty} \xi_+^{2n}
= -\frac{2\sqrt{3}t \tau \eta_{\tau s} q_x' \delta_{\tau \tau'} \delta_{ss'}}{1 + \eta_{\tau s}^2}
= \frac{2\sqrt{3}t |\tau\rangle |\eta_{\tau s}\rangle}{1 + \eta_{\tau s}^2} q_x' \delta_{\tau \tau'} \delta_{ss'}.
\] (S33)
Above in the last step, we have used the facts \( \eta_{rs} = -\tau_s \eta_{rs} \) and \( \tau^z = 1 \). Also choosing the basis to be \( (|\Psi_{11}\rangle, |\Psi_{1-1}\rangle, |\Psi_{-11}\rangle, |\Psi_{-1-1}\rangle)^\top \), then \( \mathcal{H}_{\text{zigzag,1}} \) can be expressed in terms of the Pauli matrices as

\[
\mathcal{H}_{\text{zigzag,1}} = 2\sqrt{3}\xi|\eta_{rs}|q'_x \tau_0 s_z. \tag{S34}
\]

For the third term, \( \mathcal{H}_{2,3} = -2\sqrt{3}\lambda_s q'_x \tau_0 s_z \), its matrix form reads

\[
\mathcal{H}_{2,3} = \tau_0 \otimes s_z \otimes \begin{pmatrix}
2\sqrt{3}\lambda_s q'_x & 0 & 0 & 0 & 0 & 0 & \cdots \\
0 & -2\sqrt{3}\lambda_s q'_x & 0 & 0 & 0 & 0 & \cdots \\
0 & 0 & 2\sqrt{3}\lambda_s q'_x & 0 & 0 & 0 & \cdots \\
0 & 0 & 0 & -2\sqrt{3}\lambda_s q'_x & 0 & 0 & \cdots \\
0 & 0 & 0 & 0 & 2\sqrt{3}\lambda_s q'_x & 0 & \cdots \\
0 & 0 & 0 & 0 & 0 & -2\sqrt{3}\lambda_s q'_x & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots 
\end{pmatrix}. \tag{S35}
\]

Its contribution to the boundary Hamiltonian can be similarly determined, which takes the form

\[
(\mathcal{H}_{\text{zigzag,2}})_{\tau s, \tau's'} = \langle \Psi_{\tau s} | \mathcal{H}_{2,3} | \Psi_{\tau's'} \rangle = 2\sqrt{3}\lambda_s \eta_{rs} q'_x (\eta_{rs}^2 - 1)N^2 \sum_{n=0}^{\infty} \xi_n^{2n} \delta_{\tau \tau'} \delta_{s s'}
\]

\[
= 2\sqrt{3}\lambda_s \eta_{rs}^2 - 1)q'_x \tau_0 s_z. \tag{S36}
\]

Also in terms of the Pauli matrices, its form can be expressed as

\[
\mathcal{H}_{\text{zigzag,2}} = \frac{2\sqrt{3}\lambda_s (\eta_{rs}^2 - 1)}{1 + \eta_{rs}^2} q'_x \tau_0 s_z. \tag{S37}
\]

A combination of the two contributions gives the full expression for the linear momentum term in the boundary Dirac Hamiltonian. For the chemical potential term, its contribution is also simply

\[
\mathcal{H}_{\text{zigzag,3}} = -\mu \tau_z s_0. \tag{S38}
\]

Let us now analyze the contribution from the last piece, the pairing term \( \mathcal{H}_{2,5} = -[\Delta_0 + 2\Delta_2 (-1 - \sqrt{3}q'_x \cos \frac{3\delta}{2})] \tau_y s_y \sigma_0 \). Its explicit matrix form is

\[
\mathcal{H}_{2,5} = \begin{pmatrix}
-(\Delta_0 - 2\Delta_2) \tau_y s_y & 0 & \sqrt{3}\Delta_2 q'_x \tau_y s_y & 0 & \cdots \\
0 & -(\Delta_0 - 2\Delta_2) \tau_y s_y & 0 & \sqrt{3}\Delta_2 q'_x \tau_y s_y & \cdots \\
\sqrt{3}\Delta_2 q'_x \tau_y s_y & 0 & -(\Delta_0 - 2\Delta_2) \tau_y s_y & 0 & \cdots \\
0 & \sqrt{3}\Delta_2 q'_x \tau_y s_y & 0 & -(\Delta_0 - 2\Delta_2) \tau_y s_y & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots 
\end{pmatrix}. \tag{S39}
\]

Its contribution to the boundary Hamiltonian is

\[
(\mathcal{H}_{\text{zigzag,4}})_{\tau s, \tau's'} = \langle \Psi_{\tau s} | \mathcal{H}_{2,5} | \Psi_{\tau's'} \rangle = -(\Delta_0 - 2\Delta_2) (\tau_y)_{\tau s ^{s s'}} + \sqrt{3}\Delta_2 q'_x (\tau_y)_{\tau'r ^{s s'}} \left(\sum_{n=1}^{+\infty} 2[\psi_{n B} \psi_{(n+1) B} + \psi_{(n+1) A} \psi_{(n+2) A}] \right)^n
\]

\[
= -(\Delta_0 - 2\Delta_2) (\tau_y)_{\tau' ^{(s s')}}. \tag{S40}
\]

In the last step, we have used the fact that the products \( \psi_{n B} \psi_{(n+1) B} \) and \( \psi_{n A} \psi_{(n+1) A} \) are always zero as \( \psi_{(2n+1) A} = \psi_{2n+1} = 0 \). In terms of the Pauli matrices,

\[
\mathcal{H}_{\text{zigzag,4}} = -(\Delta_0 - 2\Delta_2) \tau_y s_y. \tag{S41}
\]

Taking all contribution together, we reach the final expression for the boundary Hamiltonian for the upper zigzag edge, which reads

\[
\mathcal{H}_{\text{zigzag}} = \sum_{i=1}^{4} \mathcal{H}_{\text{zigzag},i} = v' q'_x \tau_0 s_z - \mu \tau_z s_0 - (\Delta_0 - 2\Delta_2) \tau_y s_y. \tag{S42}
\]

\[
\sum_{n=0}^{\infty} \xi_n^{2n} \delta_{\tau \tau'} \delta_{s s'}
\]
When $\lambda_{so} \ll t$, one can do an expansion of $\eta_{rs}$ about $\lambda_{so}/t$. Only keeping the leading-order term, the result is

$$|\eta_{rs}| = \frac{4t\lambda_{so}^2}{\lambda_{so}(\sqrt{t^2(\lambda_{so}^2 + 16\lambda_{so}^2 - t^2)})} \approx \frac{4t\lambda_{so}^2}{\lambda_{so}(t^2 + 8\lambda_{so}^2 - t^2)} = \frac{t}{2\lambda_{so}}. \quad (S44)$$

When $\lambda_{so} \ll t$, $|\eta_{rs}| \gg 1$, so $\eta_{rs}^2 \pm 1 \approx \eta_{rs}^2$, one finds

$$v' = \frac{2\sqrt{3}t|\eta_{rs}| + 2\sqrt{3}\lambda_{so}(\eta_{rs}^2 - 1)}{1 + \eta_{rs}^2} \approx \frac{2\sqrt{3}t|\eta_{rs}| + 2\sqrt{3}\lambda_{so}\eta_{rs}^2}{\eta_{rs}^2} \approx 6\sqrt{3}\lambda_{so}. \quad (S45)$$

In the limit $\mu = 0$, the boundary Hamiltonian reduces to the form of Eq.(9) in the main text. By comparing the analytical results with the numerical results, we find that the above low-energy boundary Hamiltonian gives a very accurate description of the physics on the zigzag edge.

**II. TWO-DIMENSIONAL HONEYCOMB-LATTICE TOPOLOGICAL INSULATORS IN PROXIMITY TO D-WAVE SUPERCONDUCTORS**

In the main text, we have used the isotropic extended s-wave pairing to illustrate the physics. To show explicitly that the physics does not rely on a specific pairing type, in this section we consider the d-wave pairing, a pairing type widely believed to be relevant to high-$T_c$ cuprate-based superconductors. On a honeycomb lattice, the pairing amplitude of the d-wave pairing follows the pattern $\Delta_{ij} = \Delta \cos 2\theta_{ij}$, with $\theta_{ij}$ denoting the angle that the bond vector $d_{ij}$ is in regard to the $x$ direction. Accordingly, the Kane-Mele model with d-wave pairing up to the next-nearest neighbors reads

$$H_{\text{BDG}}(k) = t(2\cos\frac{\sqrt{3}k_x}{2} \cos \frac{k_y}{2} + \cos k_y)\tau_z s_0 \sigma_x - t(2\cos\frac{\sqrt{3}k_x}{2} \sin \frac{k_y}{2} - \sin k_y)\tau_z s_0 \sigma_y$$

$$+ 2\lambda_{so}(\sin \sqrt{3}k_x - 2\sin\frac{\sqrt{3}k_x}{2} \cos \frac{3k_y}{2})\tau_0 s_z \sigma_z - \mu \tau_z s_0 \sigma_0$$

$$- \Delta_1(\cos\frac{\sqrt{3}k_x}{2} \cos \frac{k_y}{2} - \cos k_y)\tau_y s_y \sigma_x + \Delta_1(\cos\frac{\sqrt{3}k_x}{2} \sin \frac{k_y}{2} + \sin k_y)\tau_y s_y \sigma_y$$

$$- 2\Delta_2(\cos\frac{\sqrt{3}k_x}{2} \cos \frac{3k_y}{2})\tau_y s_y \sigma_0. \quad (S46)$$

Similar to the extended s-wave pairing, we find that the nearest-neighbor pairing also has a negligible effect to the helical edge states, and only the next-nearest-neighbor pairing can open a gap to the boundary Dirac points, as shown in Fig. S1. Therefore, below we also set $\Delta_1 = 0$ for simplicity. In parallel to the extended s-wave pairing case, we first derive the corresponding low-energy boundary Hamiltonian for both beard and zigzag edges, and then numerically show the realization of Majorana Kramers pairs at the sublattice domain walls once the topological criterion is fulfilled.

**A. Low-energy boundary Hamiltonian for the beard edge**

Compared to the extended s-wave pairing case, since only the pairing term has been changed, what we need to concern is just the change of Dirac mass. For the beard edge, as aforementioned the expansion of the Hamiltonian is around $k_x = 0$. Also only
FIG. S1. (Color online) Energy spectrum for the Kane-Mele model with d-wave pairing. A cylindrical geometry is considered, with periodic boundary condition in the $x$ direction and open boundary condition in the $y$ direction. The upper $y$-normal boundary is a beard edge, and the lower $y$-normal boundary is a zigzag edge. In (a) and (b), $t = 1, \lambda_{so} = 0.1, \mu = 0$. In (a), $\Delta_1 = 0.1$ and $\Delta_2 = 0$, the boundary Dirac points at time-reversal invariant momentums turn out to be robust against the nearest-neighbor pairing. In (b), $\Delta_1 = 0$ and $\Delta_2 = 0.1$, the boundary Dirac points are gapped by the next-nearest-neighbor pairing.

remaining terms up to the linear order in momentum, the Hamiltonian reads

$$
H_{\text{BdG}}(q_x, k_y) = t(2 \cos \frac{k_y}{2} + \cos k_y)\tau_z s_0 \sigma_x - t(2 \sin \frac{k_y}{2} - \sin k_y)\tau_z s_0 \sigma_y
+ 2\sqrt{3}\lambda_{so} q_x (1 - \cos \frac{3k_y}{2})\tau_0 s_x \sigma_z - \mu \tau_z s_0 \sigma_0
- 2\Delta_2 (1 - \cos \frac{3k_y}{2})\tau_y s_y \sigma_0,
$$

(S47)

where the last line corresponds to the pairing term at the neighborhood of $k_x = 0$. Focusing on the last line, its matrix form in the underlying basis $\Psi_{q_x} = (c_1.A,q_x, c_1.B,q_x, c_2.A,q_x, c_2.B,q_x, \ldots, c_n.A,q_x, c_n.B,q_x, \ldots)^T$ is

$$
H_{dSC} =
\begin{pmatrix}
-2\Delta_2 \tau_y s_y & 0 & \Delta_2 \tau_y s_y & 0 & \cdots \\
0 & -2\Delta_2 \tau_y s_y & 0 & \Delta_2 \tau_y s_y & \cdots \\
\Delta_2 \tau_y s_y & 0 & -2\Delta_2 \tau_y s_y & 0 & \cdots \\
0 & \Delta_2 \tau_y s_y & 0 & -2\Delta_2 \tau_y s_y & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}.
$$

(S48)

Also taking this term as a perturbation and projecting it onto the subspace spanned by the four eigenvectors $|\Psi_{\tau s}\rangle$, where

$$
|\Psi_{\tau s}\rangle = |\tau_z = \tau\rangle \otimes |s_z = s\rangle \otimes \frac{\sqrt{3}}{2} (1, 0, -\frac{1}{2}, 0, \ldots, (-\frac{1}{2})^{(n-1)}, 0, \ldots)^T,
$$

(S49)

one finds that its contribution is

$$
(H_{\text{beard,3}})_{\tau s, \tau' s'} = \langle \Psi_{\tau s} |H_{dSC}| \Psi_{\tau' s'}\rangle
= -2\Delta_2 (\tau_y)_{\tau\tau'} (s_y)_{ss'} - \Delta_2 (\tau_y)_{\tau\tau'} (s_y)_{ss'}
= -3\Delta_2 (\tau_y)_{\tau\tau'} (s_y)_{ss'}.
$$

(S50)

In terms of the Pauli matrices, its form is

$$
H_{\text{beard,3}} = -3\Delta_2 \tau_y s_y.
$$

(S51)

Replacing the Dirac mass term in Eq. (S17) by the above Dirac mass term, one gets

$$
H_{\text{beard}} = v q_x \tau_0 s_z - \mu \tau_z s_0 - 3\Delta_2 \tau_y s_y.
$$

(S52)

This is the low-energy boundary Hamiltonian for the beard edge when the pairing is d-wave type.
B. Low-energy boundary Hamiltonian for the zigzag edge

For zigzag edge and d-wave pairing, an expansion of the Hamiltonian around \( k_x = \pi/\sqrt{3} \) up to the linear order in momentum gives

\[
H_{\text{BdG}}(q'_x, k_y) = t(-\sqrt{3}q'_x \cos \frac{k_y}{2} + \cos k_y)\tau_z s_0 \sigma_x + t(\sqrt{3}q'_x \sin \frac{k_y}{2} + \sin k_y)\tau_z s_0 \sigma_y \\
+ 2\lambda_{so}(\sqrt{3}q'_x - 2\cos \frac{3k_y}{2})\tau_0 s_z \sigma_z - \mu \tau_z s_0 \sigma_0 \\
- 2\Delta_2(-1 + \sqrt{3}q'_x \cos \frac{3k_y}{2})\tau_y s_y \sigma_0.
\]

(S53)

where the last line corresponds to the pairing term at the neighborhood of \( k_x = \pi/\sqrt{3} \).

In the basis \( \Psi_{q'_x} = (c_1, c_2, c_3, ..., c_n, B, q'_x, c_5, ..., c_5) \), the matrix form of the pairing term reads

\[
H_{dSC} = \begin{pmatrix}
2\Delta_2 \tau_y s_y & 0 & \sqrt{3}/2 \Delta_2 q'_x \tau_y s_y & 0 & \cdots \\
0 & 2\Delta_2 \tau_y s_y & 0 & \sqrt{3}/2 \Delta_2 q'_x \tau_y s_y & \cdots \\
\sqrt{3}/2 \Delta_2 q'_x \tau_y s_y & 0 & 2\Delta_2 \tau_y s_y & 0 & \cdots \\
0 & \sqrt{3}/2 \Delta_2 q'_x \tau_y s_y & 0 & 2\Delta_2 \tau_y s_y & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}.
\]

(S54)

Also taking this term as a perturbation and projecting it onto the subspace spanned by the four eigenvectors \( |\Psi_{s_\tau}\rangle \), where

\[
|\Psi_{s_\tau}\rangle = |\tau_z = \tau\rangle \otimes |s_z = s\rangle \otimes N(\eta_{rs}, 1, 0, \xi_{rs}, \xi^2_{rs}, \xi^2_{rs})\]

(S55)

with \( \xi, \eta \) and \( N \) given by Eqs. (S27), (S28) and (S31), respectively, one finds that its contribution is

\[
\langle H_{\text{zigzag},5} \rangle_{s_\tau,s'_\tau} = \langle \Psi_{s_\tau}|H_{dSC}|\Psi_{s'_\tau}\rangle = 2\Delta_2(\tau_y)|s_y|s'_y.
\]

(S56)

In terms of the Pauli matrices, its form can be expressed as

\[
H_{\text{zigzag},5} = 2\Delta_2 \tau_y s_y.
\]

(S57)

Replacing the Dirac mass term in Eq. (S17) by the above Dirac mass term, one gets

\[
H_{\text{zigzag}} = v'q'_x \tau_0 s_z - \mu \tau_z s_0 + 2\Delta_2 \tau_y s_y.
\]

(S58)

This is the low-energy boundary Hamiltonian for the zigzag edge when the pairing is d-wave type.

C. Majorana Kramers pairs at sublattice domain walls on the upper boundary

Let us focus on the special case with \( \mu = 0 \). According to the low-energy boundary Hamiltonian for both beard and zigzag edges, one knows that if the upper boundary becomes nonuniform and consists of two parts which respectively terminate at A and B sublattices, the corresponding low-energy boundary Hamiltonian, due to the further breaking of translation symmetry in the \( x \) direction, will become

\[
H = -iv(x)\partial_x \tau_0 s_z + m(x)\tau_y s_y,
\]

(S59)

where \( v(x) = v, m(x) = -3\Delta_2 \) if the part corresponds to a beard edge, and \( v(x) = v', m(x) = 2\Delta_2 \) if the part corresponds to a zigzag edge. The velocities in both parts have the same sign, but the Dirac masses have opposite signs, as a result, the sublattice domain walls correspond to domain walls of Dirac mass as long as \( \Delta_2 \neq 0 \). This conclusion suggests that the sublattice domain walls will bind Majorana Kramers pairs if the next-nearest-neighboring pairing is finite. Through numerical calculations, we confirm the appearance of Majorana Kramers pairs at the sublattice domain walls, as shown in Fig. S2. The results in this section demonstrate that the emergence of Majorana zero modes at sublattice domain walls is not restricted to certain specific pairing type.
FIG. S2. (Color online) Majorana Kramers pairs at sublattice domain walls on the upper boundary. The lattice geometry is cylindrical with periodic boundary condition in the $x$ direction except for the upper most beard-edge part (left and right edges are considered to be connected in our numerical calculations). Throughout this work, the same boundary conditions are applied to all similar lattice geometries, below the boundary conditions will no longer be emphasized when similar lattice geometries are present. In (a) and (b), $t = 1$, $\lambda_{so} = 0.1$, $\mu = 0$, $\Delta_1 = 0$, $\Delta_2 = 0.15$, and the considered lattice geometry and size are shown explicitly. The insets on top of the underlying lattices correspond to the energy spectra. Here we have only shown the part of eigenvalues closest to zero energy. The middle four dots in red indicate the existence of two Majorana Kramers pairs. The shade of red color on the lattice sites reflect the weight of the probability density ($|\psi(x, y)|^2$) of Majorana Kramers pairs.

FIG. S3. (Color online) The evolution of boundary energy gap with respect to $\mu$. A cylindrical geometry is considered, with periodic boundary condition in the $x$ direction and open boundary condition in the $y$ direction. The upper $y$-normal boundary is a beard edge, and the lower $y$-normal boundary is a zigzag edge. Here the extended s-wave pairing is considered. In (a)-(c), $t = 1$, $\lambda_{so} = 0.1$, $\Delta_0 = \Delta_2 = 0.3$, $\Delta_1 = 0$. (a) $\mu = 0.2$, the mid-gap red lines show the existence of a finite gap in the boundary energy spectrum. (b) $\mu = 0.345$, the boundary energy gap vanishes, corresponding to the critical point of a boundary topological phase transition. (c) $\mu = 0.45$, a gap is reopened in the boundary energy spectrum.

III. THE IMPACT OF FINITE CHEMICAL POTENTIAL ON THE TOPOLOGICAL CRITERION

Above we have restricted to the $\mu = 0$ case for illustration. As the robustness of Majorana Kramers pairs is protected by non-spatial time-reversal symmetry and particle-hole symmetry and the chemical potential term does not break these two symmetries, the Majorana Kramers pairs will remain robust as long as the chemical potential is lower than a critical value. Before proceeding, it is worth noting that in this work we consider that the superconductivity in the two-dimensional topological insulator is induced by proximity effect. Accordingly, the chemical potential is not required to cross the bulk conduction or valence band to guarantee a metallic normal state to achieve superconductivity.
FIG. S4. (Color online) The effect of chemical potential on Majorana Kramers pairs. In (a1)-(c2), $t = 1$, $\lambda_{so} = 0.1$, $\Delta_0 = \Delta_2 = 0.3$, $\Delta_1 = 0$. In (a1) and (a2), $\mu = 0.1$, the wave functions of Majorana Kramers pairs remain well-localized so their energy splitting (see red dots in (a2)) induced by the overlap of wave functions in the considered finite-size system remains small. In (b1) and (b2), $\mu = 0.2$, the increase of $\mu$ reduces the boundary energy gap. As a result, the localization of the wave functions of Majorana Kramers pairs becomes relatively poorer and the energy splitting increases due to the finite size of the geometry. In (c1) and (c2), $\mu = 0.4$, no Majorana Kramers pairs are found as the chemical potential is beyond the critical value. The dots in cyan correspond to the lowest-energy excitations. One can see from (c1) that their wave functions are quite uniform on the boundary edge of the upper boundary.

Since the Majorana Kramers pairs have codimension $d_c = 2$, the critical chemical potential corresponds to the value at which a boundary topological phase transition occurs. At the critical point of a boundary topological phase transition, the boundary energy gap vanishes, while the bulk energy gap can remain open. We can first give an estimate of the critical value through the low-energy boundary Hamiltonian. According to Eqs. (S17) and (S42), the Dirac mass changes sign from $k_x = 0$ to $k_x = \pi/\sqrt{3}$ when $|\Delta_2| > |\Delta_0|/\sqrt{2} > 0$. It indicates that there exists a node between 0 and $\pi/\sqrt{3}$. Furthermore, as the $\Delta_2$-term cannot open a gap at $k_x = 0$ and the $\Delta_0$-term opens an equal gap at $k_x = 0$ and $k_x = \pi/\sqrt{3}$, according to the tight-binding form of the pairing term in Eq. (S1), the Dirac mass induced by the on-site and next-nearest-neighbor pairings on the boundary can be approximated as

$$m(k_x) \approx -\Delta_0 + 2\Delta_2(\cos \sqrt{3}k_x - \cos \frac{\sqrt{3}}{2}k_x).$$

(S60)

For the parameters considered in the main text, $\Delta_0 = \Delta_2 = 0.3$, the node determined by the above formula is located at $k_{x,n} \approx 0.73$. Since this momentum is closer to $k_x = 0$ than to $k_x = \pi/\sqrt{3}$, we can focus on the low-energy boundary Hamiltonian for the boundary edge shown in Eq. (S17), whose energy spectrum is

$$E = \pm \sqrt{(3\sqrt{3}\lambda_{so}q_x \pm \mu)^2 + m^2(q_x)}.$$  

(S61)

Accordingly, the critical chemical potential is approximately given by

$$\mu_c \approx 3\sqrt{3}\lambda_{so}k_{x,n} \approx 3.8\lambda_{so}.$$  

(S62)
For \( \lambda_{so} = 0.1, \mu_c \approx 0.38 \). In Fig S3(b), the evolution of boundary energy gap with respect to \( \mu \) is shown. Fig S3(b) shows that the precise value of \( \mu_c \) for the given set of parameters is 0.345, quite close to the estimated value. The formula in Eq. (S62) indicates that a stronger spin-orbit coupling admits a larger range of chemical potential within which the sublattice domain walls can host Majorana Kramers pairs.

In Fig S4, the numerical results confirm that the Majorana Kramers pairs are robust against the increase of chemical potential as long as its value remains lower than the critical value.

IV. SUBLATTICE-SENSITIVE MAJORANA MODES IN TIME-REVERSAL SYMMETRY BROKEN SYSTEMS

So far, we have restricted to time-reversal invariant cases. In this section, we consider the introduction of an in-plane magnetic field to break the time-reversal symmetry. To be specific, we consider that the magnetic field is applied in the \( x \) direction, in parallel to the domain walls on the upper boundary. The magnetic field will contribute a Zeeman splitting term of the form \( B_z \tau_z s_z \sigma_0 \) (g-factor and Bohr magneton are absorbed in \( B_z \) for notational simplicity) to the Hamiltonian. Also treating this term as a perturbation, since this term contains \( \sigma_0 \) in the sublattice subspace, one can easily find that it will contribute a Dirac mass term of the form \( B_z \tau_z s_z \) for both beard and zigzag edges. For generality, let us assume that the Dirac mass induced by superconductivity on the beard edge is of the form \( m_b \tau_y s_y \) and that on the zigzag edge is of the form \( m_z \tau_y s_y \). Taking into account the contribution from the Zeeman field, the corresponding low-energy boundary Hamiltonians are

\[
H_{beard} = v q_z \tau_0 s_z - \mu \tau_z s_0 + m_b \tau_y s_y + B_z \tau_z s_z, \\
H_{zigzag} = v' q_z' \tau_0 s_z - \mu \tau_z s_0 + m_z \tau_y s_y + B_z \tau_z s_x.
\]

(S63)

Similar to the chemical potential, the Zeeman field will induce a boundary topological phase transition when it induces a gap closure in the boundary energy spectrum. According to the boundary energy spectrum,

\[
E_{beard}(q_z) = \pm \sqrt{v^2 q_z^2 + \mu^2 + m_b^2 + B_z^2 \pm 2 \sqrt{\mu^2 v^2 q_z^2 + B_z^2 (\mu^2 + m_b^2)}}, \\
E_{zigzag}(q_z') = \pm \sqrt{v'^2 q_z'^2 + \mu^2 + m_z^2 + B_z^2 \pm 2 \sqrt{\mu^2 v'^2 q_z'^2 + B_z^2 (\mu^2 + m_z^2)}}.
\]

(S64)

For both beard and zigzag edges, the boundary energy gaps will get closed at the time-reversal invariant momentum, i.e., \( q_x = 0, q_z' = 0 \). For the beard edge, the closure of boundary energy gap occurs when \( |B_z| = B_{b,c} \equiv \sqrt{\mu^2 + m_b^2} \). For the zigzag edge, the condition is similar, that is, \( |B_{z,c} = B_{z,c} \equiv \sqrt{\mu^2 + m_z^2} \). The critical conditions for the two types of edges indicate that if the Zeeman field is chosen to satisfy \( \min \{B_{b,c}, B_{z,c}\} < B_z < \max \{B_{b,c}, B_{z,c}\} \), the system will enter a new topological phase on the boundary. For this new topological phase, the Dirac mass of sublattice domain walls will become dominated by Zeeman field on one side and by superconductivity on the other side. Accordingly, one sublattice domain wall will change to host a single Majorana zero mode, instead of a Majorana Kramers pair due to the breaking of time-reversal symmetry.

For \( \lambda_{so} = 0.1, \mu_c \approx 0.38 \). In Fig S3(b), the evolution of boundary energy gap with respect to \( \mu \) is shown. Fig S3(b) shows that the precise value of \( \mu_c \) for the given set of parameters is 0.345, quite close to the estimated value. The formula in Eq. (S62) indicates that a stronger spin-orbit coupling admits a larger range of chemical potential within which the sublattice domain walls can host Majorana Kramers pairs.

In Fig S4, the numerical results confirm that the Majorana Kramers pairs are robust against the increase of chemical potential as long as its value remains lower than the critical value.

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\[
H_{beard} = v q_z \tau_0 s_z - \mu \tau_z s_0 + m_b \tau_y s_y + B_z \tau_z s_z, \\
H_{zigzag} = v' q_z' \tau_0 s_z - \mu \tau_z s_0 + m_z \tau_y s_y + B_z \tau_z s_x.
\]

(S63)

Similar to the chemical potential, the Zeeman field will induce a boundary topological phase transition when it induces a gap closure in the boundary energy spectrum. According to the boundary energy spectrum,

\[
E_{beard}(q_z) = \pm \sqrt{v^2 q_z^2 + \mu^2 + m_b^2 + B_z^2 \pm 2 \sqrt{\mu^2 v^2 q_z^2 + B_z^2 (\mu^2 + m_b^2)}}, \\
E_{zigzag}(q_z') = \pm \sqrt{v'^2 q_z'^2 + \mu^2 + m_z^2 + B_z^2 \pm 2 \sqrt{\mu^2 v'^2 q_z'^2 + B_z^2 (\mu^2 + m_z^2)}}.
\]

(S64)

For both beard and zigzag edges, the boundary energy gaps will get closed at the time-reversal invariant momentum, i.e., \( q_x = 0, q_z' = 0 \). For the beard edge, the closure of boundary energy gap occurs when \( |B_z| = B_{b,c} \equiv \sqrt{\mu^2 + m_b^2} \). For the zigzag edge, the condition is similar, that is, \( |B_{z,c} = B_{z,c} \equiv \sqrt{\mu^2 + m_z^2} \). The critical conditions for the two types of edges indicate that if the Zeeman field is chosen to satisfy \( \min \{B_{b,c}, B_{z,c}\} < B_z < \max \{B_{b,c}, B_{z,c}\} \), the system will enter a new topological phase on the boundary. For this new topological phase, the Dirac mass of sublattice domain walls will become dominated by Zeeman field on one side and by superconductivity on the other side. Accordingly, one sublattice domain wall will change to host a single Majorana zero mode, instead of a Majorana Kramers pair due to the breaking of time-reversal symmetry.
FIG. S6. (Color online) Majorana zero modes at sublattice domain walls. The considered lattice geometry and size are shown explicitly. Here the extended s-wave pairing is considered. In (a1)-(b2), $t = 1$, $\lambda_{so} = 0.1$, $\mu = 0.1$, $\Delta_0 = 0.2$, $\Delta_2 = 0.3$, $\Delta_1 = 0$, $B_x = 0.3$. (a1) and (b1) show the distribution of probability density profiles of Majorana zero modes, and (a2) and (b2) show the corresponding energy spectra, respectively. Here we have also only shown the part of eigenvalues closest to zero energy. The middle two dots in red in (a2) and (b2) indicate the existence of two Majorana zero modes. The shade of red color on the lattice sites in (a1) and (b1) reflect that the wave functions of Majorana zero modes are strongly localized around the sublattice domain walls.

In Fig S5, the evolution of boundary energy gap with respect to Zeeman field is shown. One can readily see that the boundary energy gap gets closed and reopened with the increase of $B_x$, in agreement with the behavior predicted by the low-energy boundary Hamiltonian. In Fig S6, the numerical results show that each sublattice domain wall hosts one Majorana zero mode when the topological criterion $\min\{B_{b,c},B_{z,c}\} < B_x < \max\{B_{b,c},B_{z,c}\}$ is fulfilled. The results indicate that Majorana zero modes at sublattice domain walls can also be achieved in time-reversal symmetry breaking systems. Here it is worth noting that if sublattice-dependent magnetism can be induced on the boundary, Majorana zero modes can be realized at the sublattice domain walls even considering a pure on-site s-wave pairing.

V. TUNING THE POSITIONS OF MAJORANA ZERO MODES BY ELECTRICALLY CONTROLLING THE LOCAL BOUNDARY POTENTIAL

In the main text as well as in Figs S2 and S6, we have shown that the positions of Majorana zero modes directly follow the change of the positions of sublattice domain walls, indicating that if the terminating sublattices can freely be added or removed, the positions of Majorana zero modes can be manipulated in a site-by-site way. Apparently, this can benefit the detection as well as the implementation of braiding Majorana zero modes. In this section, we show that the positions of Majorana zero modes can also be tuned by electrically controlling the local potential on the boundary, even though the sublattice domain walls are fixed.

To show the tunability, we add a coordinate-dependent on-site potential of the form $\sum_i V_i c_i^\dagger c_i$ to the Hamiltonian, and $V_i$ is chosen to be a nonzero constant only at the neighborhood of the sublattice domain walls. The considered lattice geometry is shown explicitly in Fig S7. For the convenience of discussion, let us label the lattice sites on the uppermost beard edge from left to right as 1, 2,...,12. In Figs S7(a1) and (a2), the on-site potential is only added to site 1. From the shade of red color on the lattice sites, it is readily found that the site having the highest weight of the probability density of Majorana zero modes becomes site 2. In Figs S7(b1) and (b2), the on-site potential is added to sites from 1 to 3. Also from the shade of red color on the lattice sites, it is readily found that the site having the highest weight is now shifted from site 2 to site 4. In Figs S7(c1) and (c2), the on-site potential is added to sites from 1 to 5. It is readily found that the site having the highest weight changes to site 6. The results demonstrate explicitly that the positions of Majorana zero modes can be manipulated site-by-site by controlling the local boundary potential.
FIG. S7. (Color online) Manipulating the positions of Majorana zero modes by electrically controlling the local potential on the uppermost beard edge. The considered lattice geometry and size are shown explicitly. Here the extended s-wave pairing is considered. In (a1)-(c2), $t = 1$, $\lambda_{so} = 0.1$, $\mu = 0$, $\Delta_0 = \Delta_2 = 0.3$, $\Delta_1 = 0$, $V = 2$. (a1)-(c1) show the distribution of probability density profiles of Majorana zero modes, with the shade of red color reflecting the weight. (a2)-(c2) are the corresponding energy spectra, also only the part of eigenvalues closest to zero energy are shown. On the uppermost beard edge, the lattice sites from left to right are labeled as 1, 2, ..., 12. In (a1) and (a2), the on-site potential $V$ is only added to the lattice site 1. In (b1) and (b2), the on-site potential $V$ is added to lattice sites from 1 to 3. In (c1) and (c2), the on-site potential $V$ is added to lattice sites from 1 to 5. A comparison of the distributions of wave functions of Majorana zero modes in (a1), (b1) and (c1) clearly shows that the positions of Majorana zero modes can be manipulated by controlling the local boundary potential.