

## Supplemental Material for “Second-Order Topological Phases in Non-Hermitian Systems”

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### I. TIGHT-BINDING HAMILTONIAN

As shown in Fig. 1 of the main text, we consider a minimal model of a second-order topological insulator on a square lattice, where each unit cell contains four sublattice degrees of freedom and asymmetric particle hoppings within each unit cell are considered. The tight-binding Hamiltonian in real-space representation is written as

$$H_{\text{tb}} = \sum_{\mathbf{R}} \left[ (t - \gamma)(c_{\mathbf{R},1}^\dagger c_{\mathbf{R},3} + c_{\mathbf{R},4}^\dagger c_{\mathbf{R},2}) + (t + \gamma)(c_{\mathbf{R},3}^\dagger c_{\mathbf{R},1} + c_{\mathbf{R},2}^\dagger c_{\mathbf{R},4}) \right. \\ \left. + (t - \gamma)(c_{\mathbf{R},3}^\dagger c_{\mathbf{R},2} - c_{\mathbf{R},1}^\dagger c_{\mathbf{R},4}) + (t + \gamma)(c_{\mathbf{R},2}^\dagger c_{\mathbf{R},3} - c_{\mathbf{R},4}^\dagger c_{\mathbf{R},1}) \right. \\ \left. + \lambda(c_{\mathbf{R},1}^\dagger c_{\mathbf{R}+\hat{x},3} + c_{\mathbf{R},4}^\dagger c_{\mathbf{R}+\hat{x},2} + \text{H.c.}) + \lambda(c_{\mathbf{R},3}^\dagger c_{\mathbf{R}+\hat{y},2} - c_{\mathbf{R},1}^\dagger c_{\mathbf{R}+\hat{y},4} + \text{H.c.}) \right], \quad (\text{S1})$$

where  $c_{\mathbf{R},i}^\dagger$  ( $i = 1, 2, 3, 4$ ) is the creation operator of a fermion at sublattice  $i$  of unit-cell site  $\mathbf{R}$ ,  $\hat{x}$  and  $\hat{y}$  denote the unit vectors along the  $x$  and  $y$  directions,  $\lambda$  is the inter-cell hopping amplitude, and  $t \pm \gamma$  denote the asymmetric intra-cell hopping amplitudes. In the momentum-space representation, the Hamiltonian  $H_{\text{tb}}$  is written as  $\mathcal{H} = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger H_{2\text{D}}(\mathbf{k}) \psi_{\mathbf{k}}$  with  $\psi_{\mathbf{k}} = (c_{\mathbf{k},1}, c_{\mathbf{k},2}, c_{\mathbf{k},3}, c_{\mathbf{k},4})^T$ . Then, we have

$$H_{2\text{D}}(\mathbf{k}) = [t + \lambda \cos(k_x)] \tau_x - [\lambda \sin(k_x) + i\gamma] \tau_y \sigma_z + [t + \lambda \cos(k_y)] \tau_y \sigma_y + [\lambda \sin(k_y) + i\gamma] \tau_y \sigma_x, \quad (\text{S2})$$

where we have set the lattice constant  $a_0 = 1$ ,  $\sigma_i$  ( $i = x, y, z$ ) is a Pauli matrix acting on the sublattice index of particles 1 and 2 as well as particles 3 and 4 within a unit cell [see Fig. 1(a) in main text], and  $\tau_i$  is a Pauli matrix acting on the space of these two pairs.

The eigenenergies of  $H_{2\text{D}}(\mathbf{k})$  are

$$E_{\pm}(\mathbf{k}) = \pm [2t^2 - 2\gamma^2 + 2\lambda^2 + 2\lambda t \cos(k_x) + 2\lambda t \cos(k_y) + 2i\lambda\gamma \sin(k_x) + 2i\lambda\gamma \sin(k_y)]^{\frac{1}{2}}, \quad (\text{S3})$$

where each of the upper and lower energy bands is two-fold degenerate. The upper and lower bands coalesce at EPs with  $E_{\pm}(\mathbf{k}_{\text{EP}}) = 0$  for  $k_x = k_y = 0$  ( $\pi$ ) or  $k_x = -k_y$ .

The bulk bands of  $H_{2\text{D}}(\mathbf{k})$  are first-order topologically trivial in the entire range of parameters, and characterized by zero Chern number [1] defined by

$$\mathcal{N} = \frac{1}{2\pi} \int_{\text{BZ}} \text{Tr}[F_{xy}(\mathbf{k})] d^2k, \quad (\text{S4})$$

where the trace is taken over the occupied bands,  $F_{xy}(\mathbf{k})$  is the non-Abelian Berry curvature

$$F_{xy}^{\alpha\beta}(\mathbf{k}) = \partial_x A_y^{\alpha\beta}(\mathbf{k}) - \partial_y A_x^{\alpha\beta}(\mathbf{k}) + i[A_x, A_y]^{\alpha\beta}. \quad (\text{S5})$$

Here  $A_\mu$  is the Berry connection

$$A_\mu^{\alpha\beta}(\mathbf{k}) = i \langle \chi_n^\alpha(\mathbf{k}) | \partial_\mu \phi_n^\beta(\mathbf{k}) \rangle, \quad (\text{S6})$$

where  $|\phi_n^\alpha(\mathbf{k})\rangle$  and  $|\chi_n^\alpha(\mathbf{k})\rangle$  are the right and left eigenstates:

$$H_{2\text{D}}(\mathbf{k}) |\phi_n^\alpha(\mathbf{k})\rangle = E_n |\phi_n^\alpha(\mathbf{k})\rangle, \quad (\text{S7})$$

$$H_{2\text{D}}^\dagger(\mathbf{k}) |\chi_n^\alpha(\mathbf{k})\rangle = E_n^* |\chi_n^\alpha(\mathbf{k})\rangle, \quad (\text{S8})$$

and  $\alpha$  denotes the band degeneracy. The right and left eigenstates satisfy the following biorthogonal normalization condition

$$\langle \chi_n^\alpha(\mathbf{k}) | \phi_m^\beta(\mathbf{k}) \rangle = \delta_{nm} \delta_{\alpha\beta}. \quad (\text{S9})$$

Numerical calculations show that  $\mathcal{N} = 0$ , indicating that the bulk bands are topologically trivial.

## II. PSEUDO-HERMITICITY

In this section, we argue that the real spectrum of our non-Hermitian system, with open boundaries along both  $x$  and  $y$  directions, results from pseudo-Hermiticity of the real-space Hamiltonian [2–5].

We rewrite the real-space Hamiltonian [see Eq. (S1)] as  $H_{\text{tb}} = H_{\text{tb}}^1 + H_{\text{tb}}^2 + H_{\text{tb}}^3$ , where

$$H_{\text{tb}}^1 = \sum_{n_x, n_y} \Phi_{n_x, n_y}^\dagger [t(\tau_x + \tau_y \sigma_y) - i\gamma(\tau_y \sigma_z - \tau_y \sigma_x)] \Phi_{n_x, n_y}, \quad (\text{S10})$$

$$H_{\text{tb}}^2 = \sum_{n_x, n_y} \Phi_{n_x, n_y}^\dagger \left[ \frac{\lambda}{2} (\tau_y \sigma_y - i\tau_y \sigma_x) \right] \Phi_{n_x, n_y+1} + \text{H.c.}, \quad (\text{S11})$$

$$H_{\text{tb}}^3 = \sum_{n_x, n_y} \Phi_{n_x, n_y}^\dagger \left[ \frac{\lambda}{2} (\tau_x + i\tau_y \sigma_z) \right] \Phi_{n_x+1, n_y} + \text{H.c.}. \quad (\text{S12})$$

Here  $n_x$  ( $n_x = 1, 2, \dots, L$ ) and  $n_y$  ( $n_y = 1, 2, \dots, L$ ) are integer-valued coordinates of unit cells in the  $x$  and  $y$  directions, respectively,  $\sigma_i$  and  $\tau_i$  ( $i = x, y, z$ ) are Pauli matrices for the degrees of freedom within a unit cell, and  $\Phi_{n_x, n_y} = (c_{n_x, n_y, A}, c_{n_x, n_y, B}, c_{n_x, n_y, C}, c_{n_x, n_y, D})^T$  is the column vector of annihilation operators with  $A, B, C$ , and  $D$  corresponding to indexes 1, 2, 3, and 4 in Fig. 1 in the main text and denoting four orbitals within a unit cell. In the basis  $\Phi = (\Phi_{1,1}, \Phi_{1,2}, \dots, \Phi_{L,L-1}, \Phi_{L,L})$ , the Hamiltonian  $H_{\text{tb}}$  is expressed as

$$H_{\text{tb}} = \Phi^\dagger H_0 \Phi, \quad (\text{S13})$$

where  $H_0$  is the matrix form of the Hamiltonian  $H_{\text{tb}}$ .

The Hamiltonian  $H_{\text{tb}}$  is pseudo-Hermitian, which satisfies

$$\eta H_0^\dagger \eta^{-1} = H_0, \quad (\text{S14})$$

where  $\eta$  is a  $4L \times 4L$  square matrix, and only contains elements  $\sigma_y$  at its anti-diagonal sites:

$$\eta = \begin{bmatrix} 0 & 0 & \dots & 0 & \sigma_y \\ 0 & 0 & \dots & \sigma_y & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \sigma_y & \dots & 0 & 0 \\ \sigma_y & 0 & \dots & 0 & 0 \end{bmatrix}. \quad (\text{S15})$$

While positivity is usually required for the definition of pseudo-Hermiticity [2–4], we do not assume the positivity here. From Eq. (S14), for any eigenenergy  $E_n$  with the eigenequation  $H_0 |\phi_n\rangle = E_n |\phi_n\rangle$ , we have

$$E_n \langle \phi_n | \eta^{-1} | \phi_n \rangle = E_n^* \langle \phi_n | \eta^{-1} | \phi_n \rangle. \quad (\text{S16})$$

Therefore, for  $\langle \phi_n | \eta^{-1} | \phi_n \rangle \neq 0$ , we have real eigenenergy  $E_n$  for the open-boundary systems, which holds for a wide range of parameters (see Fig. S1 and Fig. 3 in the main text). Note that the bulk eigenenergies can be complex in a certain range of parameters, as shown in Fig. S2.

## III. EDGE THEORY

As we argue in the main text, the mid-gap-state localization at one corner results from the interplay between symmetry  $\mathcal{M}_{xy}$  and non-Hermiticity, where each corner mode is a mutual topological state of two intersecting nontrivial edges. In this section, we develop an edge theory to explain this result. We label the four edges of a square sample as I, II, III and IV (see Fig. S3). For the sake of simplicity, we consider the case of  $\min\{\lambda, -t, \lambda + t, \gamma\} > 0$ ,  $\lambda \gg \max\{\gamma, \lambda + t\}$ , and  $\gamma > \lambda + t$ . In this case, the low-energy edge bands of the Hermitian part of  $H_{2\text{D}}(\mathbf{k})$  lie around the  $\Gamma$  point of the Brillouin zone. Therefore, we consider the continuum model of the lattice Hamiltonian [see Eq. (S2)] by expanding its wavevector  $\mathbf{k}$  to first-order around the  $\Gamma = (0, 0)$  point of the Brillouin zone, obtaining

$$\tilde{H}_{\text{cm}} = (t + \lambda) \tau_x - (\lambda k_x + i\gamma) \tau_y \sigma_z + (t + \lambda) \tau_y \sigma_y + (\lambda k_y + i\gamma) \tau_y \sigma_x. \quad (\text{S17})$$

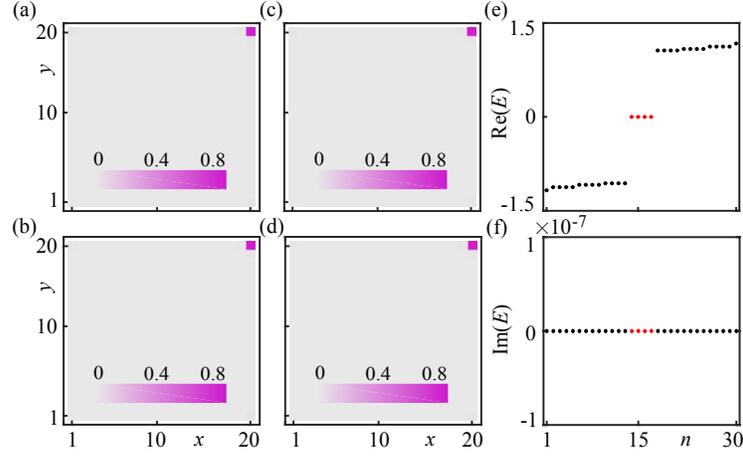


FIG. S1. (a-d) Probability density distributions  $\sum_i |\phi_{R,i,n}|^2$  ( $n$  is the index of an eigenstate and  $R$  specifies a unit cell) of four zero-energy states under the open boundary condition along both  $x$  and  $y$  directions for the  $20 \times 20$  unit cells with  $t = -0.6$ ,  $\lambda = 1.5$ , and  $\gamma = 0.4$ . All the zero-energy states are localized at the upper-right corner. (e, f) Real and imaginary parts of complex eigenenergies close to zero energy. The red dots represent the eigenenergies of the corner modes. The bulk eigenenergies for a finite-size sample are real over a wide range of parameters.

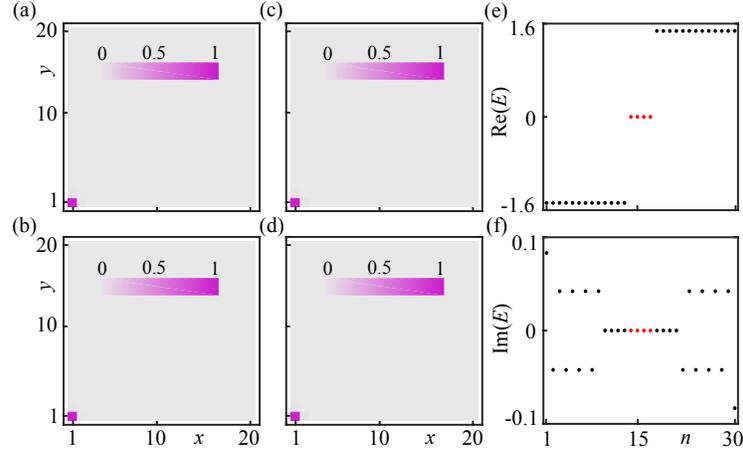


FIG. S2. (a-d) Probability density distributions of four zero-energy states under the open boundary condition along both  $x$  and  $y$  directions for the  $20 \times 20$  unit cells with  $t = 0.3$ ,  $\lambda = 1.5$ , and  $\gamma = 0.4$ . All the zero-energy states are localized at the lower-left corner. (e, f) Real and imaginary parts of complex eigenenergies close to zero energy. The red dots represent the eigenenergies of the corner modes. The bulk eigenenergies for a finite-size sample can be complex for the parameters considered here.

We first investigate the edge I of the four edges. Substituting  $k_y$  by  $-i\partial_y$ , and treating terms including  $t + \lambda$  and  $\gamma$  as perturbations (which are valid if they are relatively small), we can rewrite the Hamiltonian  $\tilde{H}_{\text{cm}}$  into the sum of the following two terms:

$$\tilde{H}_{\text{cm},1} = (t + \lambda) \tau_y \sigma_y - i\lambda \frac{\partial}{\partial y} \tau_y \sigma_x, \quad (\text{S18})$$

$$\tilde{H}_{\text{cm},2} = (t + \lambda) \tau_x - (\lambda k_x + i\gamma) \tau_y \sigma_z + i\gamma \tau_y \sigma_x, \quad (\text{S19})$$

where  $\tilde{H}_{\text{cm},1}$  is Hermitian, and  $\tilde{H}_{\text{cm},2}$  is treated as the perturbation for  $\lambda \gg \gamma, t + \lambda$ . To solve the eigenvalue equation  $\tilde{H}_{\text{cm},1} \phi_{\text{cm}}^{\text{I}}(y) = E_{\text{cm}} \phi_{\text{cm}}^{\text{I}}(y)$  with  $E_{\text{cm}} = 0$  under the boundary condition  $\phi_{\text{cm}}^{\text{I}}(+\infty) = 0$ , we can write the solution in the following form

$$\phi_{\text{cm}}^{\text{I}}(y) = \mathcal{N}_y \exp(-\alpha_{\text{I}} y) \exp(ik_x x) \chi_{\text{I}}, \quad \text{Re}(\alpha_{\text{I}}) > 0, \quad (\text{S20})$$

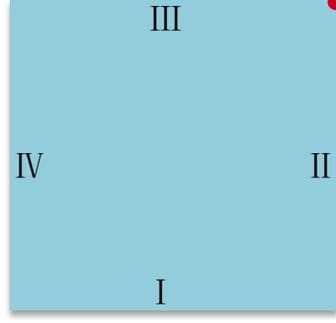


FIG. S3. Schematic illustration showing a 2D non-Hermitian SOTI in a square sample. All four zero-energy modes are localized at the upper-right corner for  $t < 0$ , and  $\gamma > 0$ . I, II, III and IV label the four edges of the lattice.

where  $\mathcal{N}_y$  is a normalization constant. The eigenvector  $\chi_I$  satisfies  $\sigma_z \chi_I = -\chi_I$  with

$$|\chi_I^1\rangle = |\tau_z = 1\rangle \otimes |\sigma_z = -1\rangle, \quad (\text{S21})$$

$$|\chi_I^2\rangle = |\tau_z = -1\rangle \otimes |\sigma_z = -1\rangle. \quad (\text{S22})$$

Then, the effective Hamiltonians for the edge I can be obtained in this basis as

$$\mathcal{H}_{\text{edge}}^I = \int_0^{+\infty} (\phi_{\text{cm}}^I)^*(y) \tilde{H}_{\text{cm},2} \phi_{\text{cm}}^I(y) dy. \quad (\text{S23})$$

Therefore, we have

$$\mathcal{H}_{\text{edge}}^I = (t + \lambda) \rho_x + (\lambda k_x + i\gamma) \rho_y, \quad (\text{S24})$$

where  $\rho_i$  ( $i = x, y, z$ ) are Pauli matrices.

The effective Hamiltonian for the edges II, III and IV can be obtained through similar procedures:

$$\mathcal{H}_{\text{edge}}^{II} = -(t + \lambda) \rho_x + (\lambda k_y + i\gamma) \rho_y, \quad (\text{S25})$$

$$\mathcal{H}_{\text{edge}}^{III} = (t + \lambda) \rho_x - (\lambda k_x + i\gamma) \rho_y, \quad (\text{S26})$$

$$\mathcal{H}_{\text{edge}}^{IV} = (t + \lambda) \rho_x + (\lambda k_y + i\gamma) \rho_y. \quad (\text{S27})$$

It is straightforward to verify that the two zero-energy bound states for edges I and III are localized at their right ends for  $\gamma > t + \lambda$  (note that each edge exhibits a zero-energy bound state for small  $\gamma$ ), while the two zero-energy bound states for edges II and IV are localized at their upper ends. Therefore, the zero-energy states are localized at the upper-right corner for  $t < 0$  and  $\gamma > 0$  (see Fig. S1).

#### IV. ROBUSTNESS AGAINST DISORDER

We now show that the zero-energy corner states are robust against disorder that preserves  $\mathcal{M}_{xy}$  symmetry and sublattice symmetry. We consider the following real-space disordered Hamiltonian:

$$\bar{H}_{\text{tb}}^1 = \sum_{n_x, n_y} \Phi_{n_x, n_y}^\dagger \left[ (t + d_1 \xi_{n_x, n_y}) (\tau_x + \tau_y \sigma_y) - i (\gamma + d_2 \zeta_{n_x, n_y}) (\tau_y \sigma_z - \tau_x \sigma_x) \right] \Phi_{n_x, n_y}, \quad (\text{S28})$$

$$\bar{H}_{\text{tb}}^2 = \sum_{n_x, n_y} \Phi_{n_x, n_y}^\dagger \left[ \frac{1}{2} (\lambda + d_3 \mu_{n_x, n_y}) (\tau_y \sigma_y - i \tau_x \sigma_x) \right] \Phi_{n_x, n_y+1} + \text{H.c.}, \quad (\text{S29})$$

$$\bar{H}_{\text{tb}}^3 = \sum_{n_x, n_y} \Phi_{n_x, n_y}^\dagger \left[ \frac{1}{2} (\lambda + d_3 \mu_{n_x, n_y}) (\tau_x + i \tau_y \sigma_z) \right] \Phi_{n_x+1, n_y} + \text{H.c.}, \quad (\text{S30})$$

where  $\xi_{n_x, n_y}$ ,  $\zeta_{n_x, n_y}$ , and  $\mu_{n_x, n_y}$  are uniform random variables distributed over  $[-1, 1]$ , while  $d_1$ ,  $d_2$ , and  $d_3$  are the corresponding disorder strength. As shown in Fig. S4 and Fig. S5 for the different values of disorder strength, the corner modes are topologically protected against disorder with the  $\mathcal{M}_{xy}$  symmetry and sublattice symmetry, unless the band gaps close. Moreover, the corner modes are well localized at one corner of a square sample [see Fig. S4(c, f, i)].

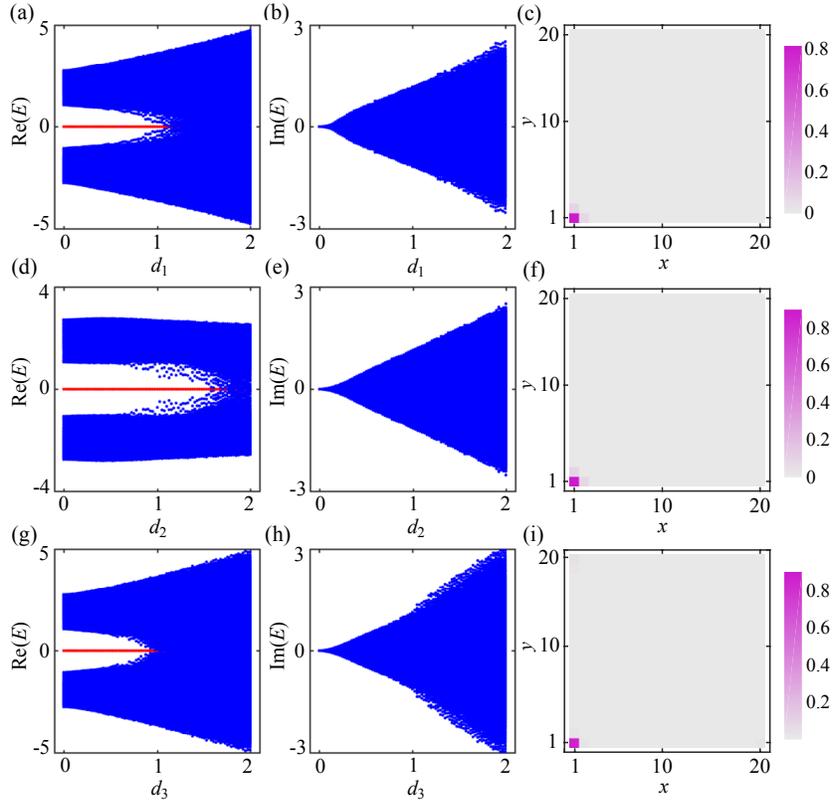


FIG. S4. Energy spectra and probability density distributions under the open boundary condition in both  $x$  and  $y$  directions (a-c) as a function of the disorder strength  $d_1$  with  $d_2 = 0$  and  $d_3 = 0$ , (d-f) as a function of the disorder strength  $d_2$  with  $d_1 = 0$  and  $d_3 = 0$ , and (g-i) as a function of the disorder strength  $d_3$  with  $d_1 = 0$  and  $d_2 = 0$ . The other parameters are chosen to be  $t = 0.6$ ,  $\lambda = 1.5$ , and  $\gamma = 0.4$ . (a, d, g) Real and (b, e, h) imaginary parts of the spectra. Red dots denote zero-energy modes. (c, f, i) Averaged probability density distributions of the four zero-energy states with  $d_1 = 0.8$ ,  $d_2 = 0.8$ , and  $d_3 = 0.8$ , respectively.

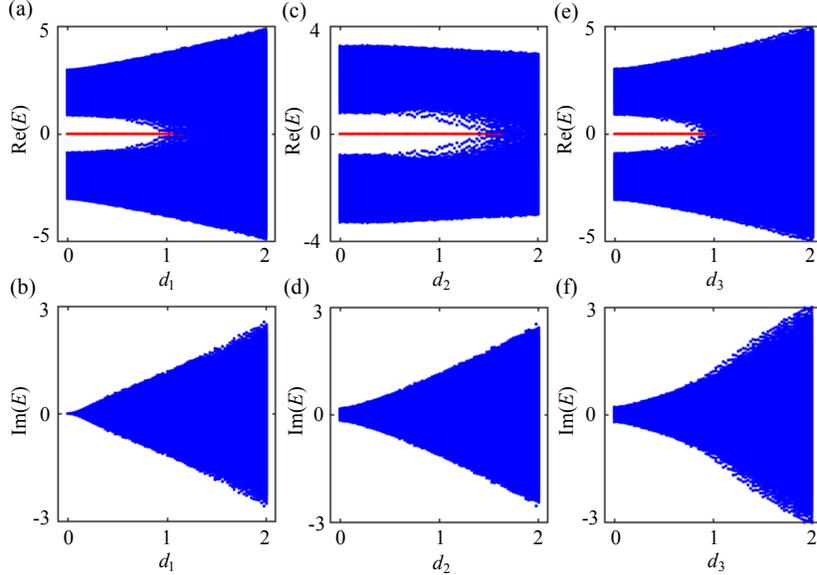


FIG. S5. Energy spectra similar to those of Fig. S4 but with the different values of disorder strength. (a, b)  $d_2 = 0.4$  and  $d_3 = 0.4$ , (c, d)  $d_1 = 0.4$  and  $d_3 = 0.4$ , and (e, f)  $d_1 = 0.4$  and  $d_2 = 0.4$ . The corner modes are topologically protected against disorder that preserves  $\mathcal{M}_{xy}$  symmetry and sublattice symmetry.

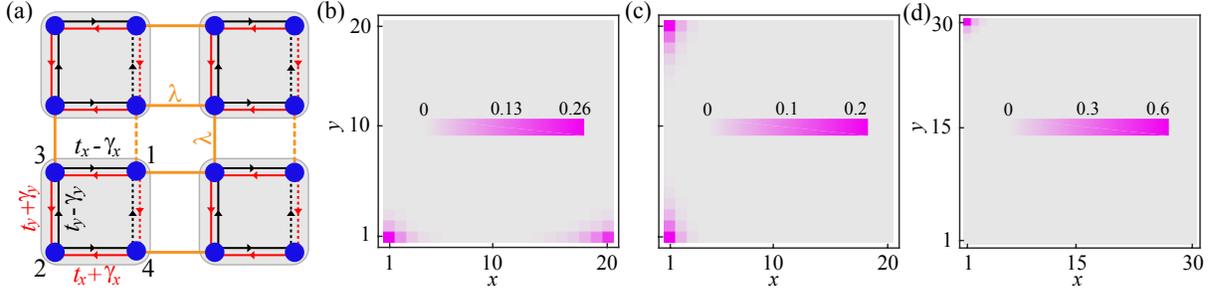


FIG. S6. (a) Real-space representation of the 2D model in Eq. (S31) on a square lattice. In contrast to the model shown in Fig. 1(a) in the main text, here we consider different amplitudes of asymmetric hopping along the  $x$  and  $y$  directions i.e.,  $\gamma_x \neq \gamma_y$ . Probability density distributions of mid-gap states under the open boundary condition along the  $x$  and  $y$  directions: (b) for  $\gamma_x = 0$  and  $\gamma_y = 0.3$ , (c) for  $\gamma_x = 0.3$  and  $\gamma_y = 0$ , and (d) for  $\gamma_x = 0.3$  and  $\gamma_y = -0.3$ . The number of unit cells is  $20 \times 20$  with  $t_x = t_y = 1.0$  and  $\lambda = 1.5$ .

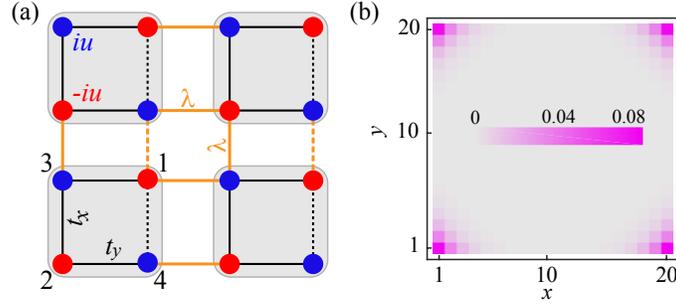


FIG. S7. (a) Real-space representation of the 2D model in Eq. (S32) in the presence of alternating on-site gain and loss (with the imaginary staggered potentials  $iu$  and  $-iu$ ) within each unit cell. The dashed lines indicate hopping terms with a negative sign. Probability density distributions of mid-gap states under the open boundary condition along the  $x$  and  $y$  directions. The number of unit cells is  $20 \times 20$  with  $u = 0.4$ ,  $t_x = t_y = 1.0$  and  $\lambda = 1.5$ .

## V. EFFECT OF A DIFFERENT TYPE OF ASYMMETRIC HOPPING AND NON-HERMITICITY ON THE LOCALIZATION OF CORNER MODES

The interplay between the mirror-rotation symmetry and non-Hermiticity leads to the localization of the mid-gap states only at one corner, as explained in the main text. However, the mid-gap modes can be localized at more than one corner when the mirror-rotation symmetry is broken. In this section, we consider the case where the mirror-rotation symmetry is broken, and study the effect of a different type of asymmetric hopping and non-Hermiticity (i.e., balanced gain and loss) on the mode localization of the mid-gap states in non-Hermitian SOTIs. Note that the effect of asymmetric hopping on the higher-order boundary modes in non-reciprocal systems has been investigated in Ref. [6].

We investigate the same lattice mode of the 2D SOTI as the one in the main text. But here we consider different amplitudes of asymmetric hopping along the  $x$  and  $y$  directions within each unit cell, i.e.,  $\gamma_x \neq \gamma_y$ , as shown in Fig. S6(a). The Bloch Hamiltonian is written as

$$\bar{H}_{2D}(\mathbf{k}) = [t_x + \lambda \cos(k_x)] \tau_x - [\lambda \sin(k_x) + i\gamma_x] \tau_y \sigma_z + [t_y + \lambda \cos(k_y)] \tau_y \sigma_y + [\lambda \sin(k_y) + i\gamma_y] \tau_y \sigma_x, \quad (\text{S31})$$

where  $\bar{H}_{2D}(\mathbf{k})$  only respects sublattice symmetry with  $\tau_z \bar{H}_{2D}(\mathbf{k}) \tau_z^{-1} = -\bar{H}_{2D}(\mathbf{k})$  for  $\gamma_x \neq \gamma_y$  for  $\gamma_x \neq \gamma_y$ . Note that 2D Hermitian SOTIs can exist even in the absence of crystalline symmetries [7].

Figure S6(b) shows the probability density distribution of mid-gap states for the larger hopping amplitude with  $(t_y + \gamma_y)$  along the  $y$  direction and the symmetric hopping along the  $x$  direction [see Fig. S6(a)]. In this case, the mid-gap states are localized at both the lower-left and lower-right corners. In contrast, for the larger hopping amplitude with  $(t_x + \gamma_x)$  along the  $x$  direction and the symmetric hopping along the  $y$  direction, the mid-gap states are localized at both the lower-left and upper-left corners, as shown in Fig. S6(c). Moreover, the mid-gap modes are localized only at the upper-left corner for the larger asymmetric hopping amplitudes with  $(t_x + \gamma_x)$  and  $(t_y - \gamma_y)$  along the  $x$  and  $y$  directions, respectively, as shown in Fig. S6(d). Therefore, the localization of corner states relies on the type of asymmetric hopping for 2D non-reciprocal lattice models.

In addition to the different type of asymmetric hopping, the second-order boundary modes in 2D systems can be localized at more than one corner in the presence of a different type of non-Hermiticity i.e., balanced gain and loss. As shown in Fig. S7(a),

we consider the alternating on-site gain and loss with symmetric particle hopping, where the imaginary staggered potentials are indicated by  $iu$  and  $-iu$ . The Bloch Hamiltonian is written as

$$\tilde{H}_{2D}(\mathbf{k}) = [t_x + \lambda \cos(k_x)] \tau_x - \lambda \sin(k_x) \tau_y \sigma_z + [t_y + \lambda \cos(k_y)] \tau_y \sigma_y + \lambda \sin(k_y) \tau_y \sigma_x - iu \tau_z. \quad (\text{S32})$$

Whereas  $\tilde{H}_{2D}(\mathbf{k})$  does not respect sublattice symmetry, it still respects pseudo-anti-Hermiticity with  $\tau_z \tilde{H}_{2D}^\dagger(\mathbf{k}) \tau_z^{-1} = -\tilde{H}_{2D}(\mathbf{k})$  [5]. As a result, the second-order topological phase survives even in the presence of the balanced gain and loss. Figure S7(b) shows the probability density distribution. In the presence of the balanced gain and loss, the mid-gap states are localized at four corners in 2D systems. In contrast to non-Hermitian SOTIs with asymmetric hopping, the eigenenergies of mid-gap states have nonzero imaginary parts as in the case for the non-Hermitian Su-Schrieffer-Heeger model with the balanced gain and loss [5].

## VI. DEGENERATE PERTURBATION THEORY

The bulk-state localization results from the non-Hermiticity due to asymmetric hopping, which can intuitively be explained using degenerate perturbation theory when  $\gamma$  is small. In this section, we consider a continuum model of the lattice Hamiltonian [see Eq. (S2)] by expanding its wavevector  $\mathbf{k}$  up to second order around the  $\Gamma = (0, 0)$  point of the Brillouin zone, obtaining  $H_{\text{cm}} = H_{\text{cm}}^1 + H_{\text{cm}}^2$ , where

$$H_{\text{cm}}^1 = \left[ t + \lambda - \frac{\lambda}{2} k_x^2 \right] \tau_x - \lambda k_x \tau_y \sigma_z + \left[ t + \lambda - \frac{\lambda}{2} k_y^2 \right] \tau_y \sigma_y + \lambda k_y \tau_y \sigma_x, \quad (\text{S33})$$

$$H_{\text{cm}}^2 = -i\gamma \tau_y \sigma_z + i\gamma \tau_y \sigma_x. \quad (\text{S34})$$

Note that  $H_{\text{cm}}^2$  can be obtained from  $H_{\text{cm}}^1$  as  $H_{\text{cm}}^2 = \bar{H}_{\text{cm}}^2 + \bar{\bar{H}}_{\text{cm}}^2$ :

$$\bar{H}_{\text{cm}}^2 = \frac{i\gamma}{\lambda} \left( \frac{\partial H_{\text{cm}}^1}{\partial k_x} + \frac{\partial H_{\text{cm}}^1}{\partial k_y} \right) = \frac{\gamma}{\lambda} ([x, H_{\text{cm}}^1] + [y, H_{\text{cm}}^1]), \quad (\text{S35})$$

$$\bar{\bar{H}}_{\text{cm}}^2 = i\gamma (k_x \tau_x + k_y \tau_y \sigma_y). \quad (\text{S36})$$

The degenerate bulk states for the Hermitian part  $H_{\text{cm}}^1$  of the Hamiltonian are denoted by  $|\phi_i^0\rangle$  ( $i = 1, 2, 3, 4$ ), and the non-Hermitian part  $H_{\text{cm}}^2$  is considered as a perturbation for  $\lambda \gg \gamma$ , and  $\mathbf{k}$  is around the  $\Gamma$  point. By applying degenerate perturbation theory [8, 9], the first-order correction to the wavefunctions  $|\phi_i^0\rangle$  for small  $\mathbf{k}$  is

$$\begin{aligned} |\phi_i^1\rangle &= \sum_{h \notin \{\phi_i^0\}} \left( \frac{\langle h | H_{\text{cm}}^2 | \phi_i^0 \rangle}{E_d^0 - E_h^0} |h\rangle + \sum_{j \neq i} \frac{\langle \phi_j^0 | H_{\text{cm}}^2 | h \rangle}{u_i - u_j} |\phi_j^0\rangle \frac{\langle h | H_{\text{cm}}^2 | \phi_i^0 \rangle}{E_d^0 - E_h^0} \right) \\ &\simeq \sum_{h \notin \{\phi_i^0\}} \left( \frac{\langle h | \bar{H}_{\text{cm}}^2 | \phi_i^0 \rangle}{E_d^0 - E_h^0} |h\rangle + \sum_{j \neq i} \frac{\langle \phi_j^0 | \bar{H}_{\text{cm}}^2 | h \rangle}{u_i - u_j} |\phi_j^0\rangle \frac{\langle h | \bar{H}_{\text{cm}}^2 | \phi_i^0 \rangle}{E_d^0 - E_h^0} \right) \\ &= \sum_{h \notin \{\phi_i^0\}} \left( \frac{\gamma}{\lambda} |h\rangle \langle h | x | \phi_i^0 \rangle + \sum_{j \neq i} \frac{\gamma^2 (E_d^0 - E_h^0) |\phi_j^0\rangle \langle h | x | \phi_i^0 \rangle \langle \phi_j^0 | x | h \rangle}{\lambda^2 (u_i - u_j)} + \right. \\ &\quad \left. \frac{\gamma}{\lambda} |h\rangle \langle h | y | \phi_i^0 \rangle + \sum_{j \neq i} \frac{\gamma^2 (E_d^0 - E_h^0) |\phi_j^0\rangle \langle h | y | \phi_i^0 \rangle \langle \phi_j^0 | y | h \rangle}{\lambda^2 (u_i - u_j)} \right) \\ &= \frac{\gamma}{\lambda} (x - \bar{x}_i) |\phi_i^0\rangle + \sum_{j \neq i} \frac{\gamma^2 (E_d^0 - E_h^0) [\langle \phi_j^0 | x^2 | \phi_i^0 \rangle - \bar{x}_j^* \bar{x}_i]}{\lambda^2 (u_i - u_j)} |\phi_j^0\rangle + \\ &\quad \frac{\gamma}{\lambda} (y - \bar{y}_i) |\phi_i^0\rangle + \sum_{j \neq i} \frac{\gamma^2 (E_d^0 - E_h^0) [\langle \phi_j^0 | y^2 | \phi_i^0 \rangle - \bar{y}_j^* \bar{y}_i]}{\lambda^2 (u_i - u_j)} |\phi_j^0\rangle \\ &\simeq \left[ \frac{\gamma}{\lambda} (x - \bar{x}_i) + \sum_{j \neq i} \frac{\gamma^2 (E_d^0 - E_h^0) [\langle \phi_i^0 | x^2 | \phi_j^0 \rangle - \bar{x}_i^* \bar{x}_j]}{\lambda^2 (u_j - u_i)} \right] |\phi_i^0\rangle + \\ &\quad \left[ \frac{\gamma}{\lambda} (y - \bar{y}_i) + \sum_{j \neq i} \frac{\gamma^2 (E_d^0 - E_h^0) [\langle \phi_i^0 | y^2 | \phi_j^0 \rangle - \bar{y}_i^* \bar{y}_j]}{\lambda^2 (u_j - u_i)} \right] |\phi_i^0\rangle, \end{aligned} \quad (\text{S37})$$

where  $E_d^0$ ,  $E_h^0$ ,  $u_i$ ,  $\bar{x}_i$  and  $\bar{y}_i$  satisfy

$$H_{\text{cm}}^1 |\phi_i^0\rangle = E_d^0 |\phi_i^0\rangle, \quad (\text{S38})$$

$$H_{\text{cm}}^1 |h\rangle = E_h^0 |h\rangle, \quad h \notin \{\phi_i^0\}, \quad (\text{S39})$$

$$u_i = \langle \phi_i^0 | H_{\text{cm}}^2 | \phi_i^0 \rangle = \langle \phi_i^0 | \bar{H}_{\text{cm}}^2 | \phi_i^0 \rangle, \quad (\text{S40})$$

$$\bar{x}_i = \sum_m \langle \phi_m^0 | x | \phi_i^0 \rangle, \quad (\text{S41})$$

$$\bar{y}_i = \sum_m \langle \phi_m^0 | y | \phi_i^0 \rangle. \quad (\text{S42})$$

Then the modified eigenstate is

$$|\phi_i\rangle = |\phi_i^0\rangle + |\phi_i^1\rangle \simeq \exp\left[\frac{\gamma}{\lambda}(x + y - \bar{x}_i - \bar{y}_i)\right] |\phi_i^0\rangle, \quad (\text{S43})$$

where  $\bar{x}_i$  and  $\bar{y}_i$  are given by

$$\bar{x}_i = \bar{x}_i - \sum_{j \neq i} \frac{\gamma(E_d^0 - E_h^0) [\langle \phi_i^0 | x^2 | \phi_j^0 \rangle - \bar{x}_i^* \bar{x}_j]}{\lambda(u_j - u_i)}, \quad (\text{S44})$$

$$\bar{y}_i = \bar{y}_i - \sum_{j \neq i} \frac{\gamma(E_d^0 - E_h^0) [\langle \phi_i^0 | y^2 | \phi_j^0 \rangle - \bar{y}_i^* \bar{y}_j]}{\lambda(u_j - u_i)}. \quad (\text{S45})$$

Equation (S43) shows that the bulk states can exponentially be localized in the non-Hermitian case, while they cannot if the perturbation Hamiltonian  $H_{\text{cm}}^2$  is Hermitian (i.e., if  $\gamma$  is pure imaginary).

## VII. BULK-STATE LOCALIZATION AND WINDING NUMBER

As explained in the main text, the winding number defined by the non-Hermitian Bloch Hamiltonian [see Eqs. (1)-(5) in the main text] cannot correctly describe the bulk-corner correspondence in the second-order topological insulator. This deviation results from the non-Bloch-wave behavior of open-boundary eigenstates of a non-Hermitian Hamiltonian [10, 11], which leads to the bulk-state localization (see Fig. 3 in the main text, and a quantitative analysis in the previous section). In order to figure out this unexpected non-Bloch-wave behavior, and precisely characterize the topological invariants for non-Hermitian systems, modified complex wavevectors, rather than real ones, are proposed for calculating the winding number [10, 11]. In this section, we discuss how to modify the topological index based on complex wavevectors.

According to Eqs. (S10) – (S13), in the basis  $\Phi = (\Phi_{1,1}, \Phi_{1,2}, \dots, \Phi_{L,L-1}, \Phi_{L,L})$ , we solve the real-space eigenequation:

$$H_0 \phi = E \phi, \quad (\text{S46})$$

where the wavefunction  $\phi$  is  $\phi = (\varphi_{1,1}, \varphi_{1,2}, \dots, \varphi_{L,L-1}, \varphi_{L,L})^T$  with  $\varphi_{n_x, n_y} = (\phi_{n_x, n_y, A}, \phi_{n_x, n_y, B}, \phi_{n_x, n_y, C}, \phi_{n_x, n_y, D})^T$ . Then, according to Eq. (S46), we have

$$T^\dagger \varphi_{n_x-1, n_y+1} + M^\dagger \varphi_{n_x, n_y} + R \varphi_{n_x, n_y+1} + M \varphi_{n_x, n_y+2} + T \varphi_{n_x+1, n_y+1} = E \varphi_{n_x, n_y+1}, \quad (\text{S47})$$

where  $R$ ,  $M$  and  $T$  are given by

$$R = t(\tau_x + \tau_y \sigma_y) - i\gamma(\tau_y \sigma_z + \tau_y \sigma_x), \quad (\text{S48})$$

$$M = \frac{\lambda}{2}(\tau_y \sigma_y - i\tau_y \sigma_x), \quad (\text{S49})$$

$$T = \frac{\lambda}{2}(\tau_x + i\tau_y \sigma_z). \quad (\text{S50})$$

To derive the eigenequation [see Eq. (S47)], we consider the trial solution

$$\varphi_{n_x, n_y} = \exp(\alpha_1 n_x + \alpha_2 n_y) \phi_0, \quad (\text{S51})$$

where  $\phi_0 = (\phi_A, \phi_B, \phi_C, \phi_D)$ . In order to preserve the symmetry  $\mathcal{M}_{xy}$ , we set  $\alpha_1 = \alpha_2 = \alpha$ . According to Eqs. (S47)–(S51), we have

$$(t - \gamma + \beta\lambda)\phi_C - (t - \gamma + \beta\lambda)\phi_D = E\phi_A, \quad (\text{S52})$$

$$[\lambda + \beta(t + \gamma)]\phi_C + [\lambda + \beta(t + \gamma)]\phi_D = \beta E\phi_B, \quad (\text{S53})$$

$$[\lambda + \beta(t + \gamma)]\phi_A + \beta(t - \gamma + \beta\lambda)\phi_B = \beta E\phi_C, \quad (\text{S54})$$

$$-[\lambda + \beta(t + \gamma)]\phi_A + \beta(t - \gamma + \beta\lambda)\phi_B = \beta E\phi_D, \quad (\text{S55})$$

where  $\beta = \exp(\alpha)$ . Therefore, we have

$$\lambda\gamma\beta^2 - (\gamma^2 - \lambda^2)\beta + t^2\beta - \gamma\lambda + (1 + \beta^2)\lambda t = \frac{\beta}{2}E^2. \quad (\text{S56})$$

Equation (S56) has two solutions  $\beta_1$  and  $\beta_2$ :

$$\beta_i = \frac{2\gamma^2 - 2\lambda^2 - 2t^2 + E^2 \pm \sqrt{(2\lambda^2 - 2\gamma^2 + 2t^2 - E^2)^2 - 8\lambda^2(t - \gamma)(\gamma + t)}}{4\lambda(\gamma + t)}. \quad (\text{S57})$$

Moreover, according to Eq. (S56), for  $E \rightarrow 0$ , we have

$$\beta_1 = -\frac{\lambda}{t + \gamma}, \quad \beta_2 = \frac{\gamma - t}{\lambda}, \quad t \in [-\sqrt{\gamma^2 + \lambda^2}, \sqrt{\gamma^2 + \lambda^2}], \quad (\text{S58})$$

$$\beta_1 = \frac{\gamma - t}{\lambda}, \quad \beta_2 = -\frac{\lambda}{t + \gamma}, \quad t \in [-\infty, -\sqrt{\gamma^2 + \lambda^2}] \cup [\sqrt{\gamma^2 + \lambda^2}, +\infty]. \quad (\text{S59})$$

Then, the state vector in Eq. (S51) at each site can be written as

$$\varphi_{n_x, n_y} = \beta_1^{n_x + n_y} \phi_0^1 + \beta_2^{n_x + n_y} \phi_0^2. \quad (\text{S60})$$

By considering the following boundary conditions

$$R(\beta_1^2 \phi_0^1 + \beta_2^2 \phi_0^2) + M(\beta_1^3 \phi_0^1 + \beta_2^3 \phi_0^2) + T(\beta_1^3 \phi_0^1 + \beta_2^3 \phi_0^2) = E(\beta_1^2 \phi_0^1 + \beta_2^2 \phi_0^2), \quad (\text{S61})$$

$$T^\dagger(\beta_1^{2L-1} \phi_0^1 + \beta_2^{2L-1} \phi_0^2) + M^\dagger(\beta_1^{2L-1} \phi_0^1 + \beta_2^{2L-1} \phi_0^2) + R(\beta_1^{2L} \phi_0^1 + \beta_2^{2L} \phi_0^2) = E(\beta_1^{2L} \phi_0^1 + \beta_2^{2L} \phi_0^2), \quad (\text{S62})$$

and relations

$$\phi_A^{(i)} = \frac{\beta_i E (\phi_C^{(i)} - \phi_D^{(i)})}{2(\lambda + t\beta + \gamma\beta)}, \quad (\text{S63})$$

$$\phi_B^{(i)} = \frac{\beta_i E (\phi_C^{(i)} + \phi_D^{(i)})}{2(t - \gamma + \lambda\beta)}, \quad (\text{S64})$$

we have

$$\beta_2^{2L-1} [2t^2 - 2\gamma^2 + 2\beta_1\lambda(\gamma + t) - E^2] = \beta_1^{2L-1} [2t^2 - 2\gamma^2 + 2\beta_2\lambda(\gamma + t) - E^2]. \quad (\text{S65})$$

According to Eq. (S65), we require that  $\beta_1$  and  $\beta_2$  satisfy

$$|\beta_1| = |\beta_2| \quad (\text{S66})$$

for a continuum spectrum, where the number of energy eigenstates is proportional to the lattice size  $L$ . Otherwise,  $\beta_1(E) = 0$  or  $2t^2 - 2\gamma^2 + 2\beta_2\lambda(\gamma + t) - E^2 = 0$  (which is independent of the lattice size  $L$ ) if  $|\beta_1| > |\beta_2|$ , and  $\beta_2(E) = 0$  or  $2t^2 - 2\gamma^2 + 2\beta_1\lambda(\gamma + t) - E^2 = 0$  (which is independent of the lattice size  $L$ ) if  $|\beta_1| < |\beta_2|$ .

By combining Eqs. (S57) and (S66), for the bulk states, we have

$$\beta_0 = |\beta_i| = \sqrt{\left| \frac{t - \gamma}{t + \gamma} \right|}. \quad (\text{S67})$$

Then, to account for the non-Bloch-wave behavior [10, 11], we replace the real wavevector  $\mathbf{k}$  with the complex one

$$\mathbf{k} = (k_x, k_y) \rightarrow \tilde{\mathbf{k}} = \mathbf{k} + i\mathbf{k}' = (k_x + ik'_x, k_y + ik'_y), \quad (\text{S68})$$

where

$$k'_x = k'_y = -\ln(\beta_0) = -\alpha_0. \quad (\text{S69})$$

Then the momentum-space Hamiltonian [see Eq. (S2)] can be expressed as

$$H_{2D}(\mathbf{k}) \rightarrow \tilde{H}(\mathbf{k}) = H(\mathbf{k} + i\mathbf{k}'). \quad (\text{S70})$$

As shown in the main text, because the Hamiltonian  $\tilde{H}(\mathbf{k})$  preserves the mirror-rotation symmetry  $\mathcal{M}_{xy}$ , we can write the Hamiltonian  $\tilde{H}(\mathbf{k})$  in a block-diagonal form with  $k_x = k_y = k$  as

$$U^{-1}\tilde{H}(k, k)U = \begin{bmatrix} \tilde{H}_+(k) & 0 \\ 0 & \tilde{H}_-(k) \end{bmatrix}, \quad (\text{S71})$$

where  $\tilde{H}_+(k)$  acts on the +1 mirror-rotation subspace, and  $\tilde{H}_-(k)$  acts on the -1 mirror-rotation subspace. The unitary transformation  $U$  is

$$U = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{bmatrix}, \quad (\text{S72})$$

and  $\tilde{H}_+(k)$  and  $\tilde{H}_-(k)$  are

$$\tilde{H}_+(k) = \sqrt{2} [t + \lambda \cos(k - i\alpha_0)] \sigma_x + \sqrt{2} [\lambda \sin(k - i\alpha_0) + i\gamma] \sigma_y, \quad (\text{S73})$$

$$\tilde{H}_-(k) = \sqrt{2} [t + \lambda \cos(k - i\alpha_0)] \sigma_x - \sqrt{2} [\lambda \sin(k - i\alpha_0) + i\gamma] \sigma_y. \quad (\text{S74})$$

We rewrite Eqs. (S73)–(S74) as

$$\tilde{H}_+(k) = \sqrt{2} (t + \gamma + \lambda\beta_0^{-1}e^{-ik}) \sigma_+ + \sqrt{2} (t - \gamma + \lambda\beta_0 e^{ik}) \sigma_-, \quad (\text{S75})$$

$$\tilde{H}_-(k) = \sqrt{2} (t - \gamma + \lambda\beta_0 e^{ik}) \sigma_+ + \sqrt{2} (t + \gamma + \lambda\beta_0^{-1}e^{-ik}) \sigma_-, \quad (\text{S76})$$

where  $\sigma_{\pm} = (\sigma_x \pm i\sigma_y)/2$ . The winding numbers for the Hamiltonians  $\tilde{H}_+(k)$  and  $\tilde{H}_-(k)$  are expressed as

$$w_+ = \frac{i}{2\pi} \int_0^{4\pi} \frac{\langle \chi_+ | \partial_k | \phi_+ \rangle}{\langle \chi_+ | \phi_+ \rangle} dk, \quad (\text{S77})$$

$$w_- = \frac{i}{2\pi} \int_0^{4\pi} \frac{\langle \chi_- | \partial_k | \phi_- \rangle}{\langle \chi_- | \phi_- \rangle} dk, \quad (\text{S78})$$

where  $|\phi_{\pm}\rangle$  and  $|\chi_{\pm}\rangle$  are the right and left eigenstates of  $\tilde{H}_{\pm}(k)$ , respectively. The integration over  $4\pi$  in Eqs. (S77)–(S78) is attributed to the  $4\pi$ -periodicity of the eigenenergies and eigenstates. Then, the total winding number is

$$w = w_+ - w_-. \quad (\text{S79})$$

### VIII. POSSIBLE EXPERIMENTAL REALIZATION

The second-order topological insulator studied here can be experimentally realized in ultracold atoms and photonic systems. In this section, we propose a possible scheme to realize a non-Hermitian second-order topological insulator in ultracold atoms in optical lattices. The idea is to combine two state-of-the-art experimental techniques: artificial gauge field and dissipation engineering. The former is used to create a  $\pi$  flux in each unit cell and the latter is used to make the hopping amplitudes asymmetric.

### A. General idea

We note that the anti-Hermitian part of the Hamiltonian can be separated into individual four-site blocks [see Eq. (S1)]. By individual we mean that the corresponding local Hamiltonians have no overlap with each other. To be specific, we consider the following four-site Hamiltonian (here we omit the notation  $R$  in operators for the sake of simplicity):

$$H_{\text{sb}} = (t + \gamma)[c_2^\dagger(c_3 + c_4) + (c_3^\dagger - c_4^\dagger)c_1] + (t - \gamma)[(c_3^\dagger + c_4^\dagger)c_2 + c_1^\dagger(c_3 - c_4)], \quad (\text{S80})$$

whose Hermitian part reads

$$H_0 = \frac{1}{2}(H_{\text{sb}} + H_{\text{sb}}^\dagger) = t[c_2^\dagger(c_3 + c_4) + (c_3^\dagger - c_4^\dagger)c_1 + (c_3^\dagger + c_4^\dagger)c_2 + c_1^\dagger(c_3 - c_4)]. \quad (\text{S81})$$

On the other hand, the anti-Hermitian part of Eq. (S80) is given by

$$\frac{1}{2}(H_{\text{sb}} - H_{\text{sb}}^\dagger) = \gamma(c_3^\dagger c_1 + c_1^\dagger c_4 + c_2^\dagger c_3 + c_2^\dagger c_4 - \text{H.c.}). \quad (\text{S82})$$

To engineer this anti-Hermitian part, we follow the method developed in Ref. [12] to use a combination of the following jump operators that describe the collective loss of two nearest-neighbor sites:

$$L_1 = \sqrt{2\gamma}(c_3 + ic_1), \quad L_2 = \sqrt{2\gamma}(c_1 + ic_4), \quad L_3 = \sqrt{2\gamma}(c_2 + ic_3), \quad L_4 = \sqrt{2\gamma}(c_2 + ic_4). \quad (\text{S83})$$

At the single-particle or mean-field level, the open-system dynamics of a single block is determined by the non-Hermitian effective Hamiltonian

$$H_{\text{eff}} = H_0 - \frac{1}{2} \sum_{j=1}^4 L_j^\dagger L_j = H_{\text{sb}} - 2\gamma \sum_{j=1}^4 c_j^\dagger c_j, \quad (\text{S84})$$

which differs from Eq. (S80) only by a background loss term proportional to  $2\gamma$ . In the following, we will discuss in detail a possible implementation of the above idea with state-of-the-art experimental techniques developed in dissipation engineering [13] and artificial gauge fields [14].

### B. Explicit implementation

We first note that, in the Hermitian limit ( $\gamma = 0$ ), there is already an ultracold-atom-based proposal in Ref. [15]. As explained therein, the Hermitian Hamiltonian can be simulated by embedding a superlattice structure into a two-dimensional  $\pi$ -flux lattice, which can be realized using a setup described in Refs. [16, 17]. Moreover, we would like to mention that a sharp (box) boundary is also available within current experimental techniques [18]. This is necessary for observing the topologically protected corner states.

Now let us move onto the asymmetric hopping amplitudes. Following the theoretical consideration sketched out above, it suffices to focus on the realization of the jump operators [Eq. (S83)]. We again follow in Ref. [12] to effectively engineer a collective loss from a combination of on-site loss of auxiliary states and their coherent coupling to the primary degrees of freedom. Without loss of generality, we now focus on the case of a single block and resonant couplings. As shown in Fig. S8, the full open-system dynamics in the rotating frame of reference can be written as

$$\dot{\rho}_t = -i[H_0 + \frac{\Omega}{2}(a_2^\dagger(c_2 + ic_4) + a_1^\dagger(c_3 + ic_1) + a_3^\dagger(c_2 + ic_3) + a_4^\dagger(c_1 + ic_4) + \text{H.c.}), \rho_t] + \kappa \sum_{j=1}^4 \mathcal{D}[a_j] \rho_t, \quad (\text{S85})$$

where  $a_j$ 's denote the annihilation operators of the particles in the auxiliary sublattice  $j$  and  $\mathcal{D}[L] \rho \equiv L \rho L^\dagger - \frac{1}{2}\{L^\dagger L, \rho\}$  is the Lindblad superoperator. In the regime  $\kappa \gg \Omega$ , we can adiabatically eliminate the fast decay modes in the auxiliary lattice [19] to obtain the following effective dynamics of the primary lattice degrees of freedom alone:

$$\dot{\rho}_t = -i[H_0, \rho_t] + 2\gamma \sum_{j=1}^4 \mathcal{D}[L_j] \rho_t, \quad (\text{S86})$$

where  $\gamma = \Omega^2/(2\kappa)$ . At the single-particle or the mean-field level, the dynamics reduces to the nonunitary evolution governed by the non-Hermitian Hamiltonian given in Eq. (S84).

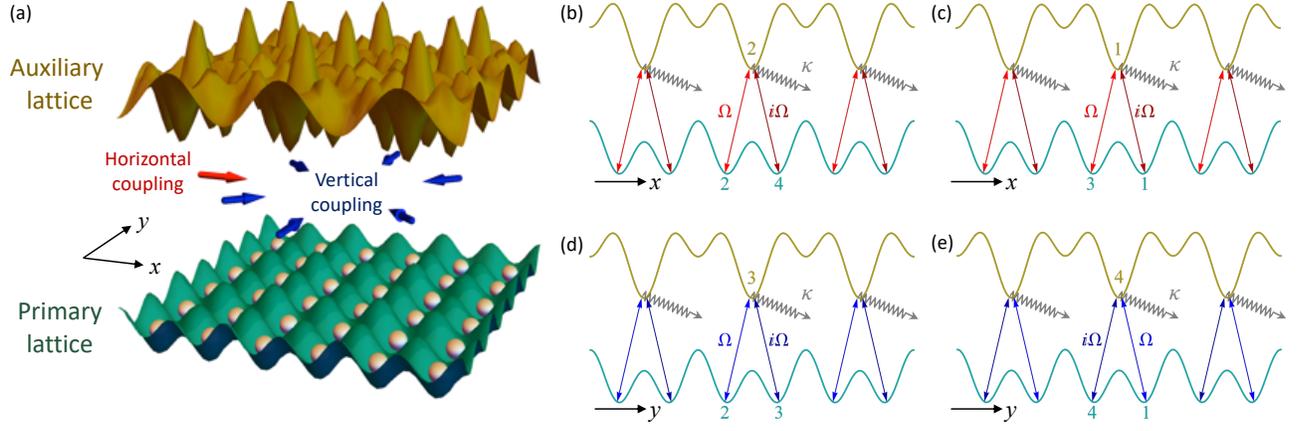


FIG. S8. (a) Schematic illustration of a proposed experimental setup. The primary lattice (green) together with a pair of Raman lasers (not shown) gives rise to a Hermitian second-order topological insulator, where the Raman lasers are used for inducing effective particle hopping. The asymmetry in hopping amplitudes is then introduced via a coherent coupling to a dissipative auxiliary lattice (yellow). In particular, the running wave (red arrow) generates the horizontal couplings shown in (b) and (c), which are the cross-sections along the  $x$  direction, containing sublattices 2, 4 and 3, 1, respectively. The other three standing waves (blue arrows) generate the vertical couplings shown in (d) and (e), which are the cross-sections along the  $y$  direction containing sublattices 2, 3 and 4, 1, respectively.

However, unlike the simple case discussed in Ref. [12], which describes a single band in one dimension, here we have two difficulties to realize the effective dynamics in Eq. (S85): (i) To ensure that an auxiliary site is only coupled to two nearest-neighbor sites, the auxiliary lattice should form a square-octagon pattern in two dimensions; (ii) We have to fine-tune the phases of couplings in the presence of a nonzero flux. Let us discuss below possible solutions to (i) and (ii).

To overcome the difficulty (i), we first note that an ideal trap with square-octagon geometry is given by

$$V_{\text{id sqoc}}(\mathbf{r}) \propto \sum_{\substack{(m,n) \in \mathbb{Z}^2 \\ s=\pm, \varsigma=0,1}} \delta\left(x - \left[\frac{s\varsigma}{4} + m\right]a\right) \delta\left(y - \left[\frac{1-\varsigma}{4}s + n\right]a\right), \quad (\text{S87})$$

which can be expanded into the Fourier series

$$V_{\text{id sqoc}}(\mathbf{r}) \propto \sum_{(m,n) \in \mathbb{Z}^2} [i^m + (-i)^m + i^n + (-i)^n] \exp\left(i \frac{2\pi}{a} [mx + ny]\right). \quad (\text{S88})$$

Here  $a$  is the lattice constant, which equals  $\lambda_1$ , the wavelength of the laser that generates the primary lattice [15]. Keeping the terms with  $|m| + |n| = 3, 4$  in Eq. (S88) followed by dropping the constants and adjusting the coefficients, we can construct a square-octagon-lattice potential as

$$V_{\text{sqoc}} \propto \left[ \cos^2 \frac{\pi(2x+y)}{a} + \cos^2 \frac{\pi(2x-y)}{a} + \cos^2 \frac{\pi(x+2y)}{a} + \cos^2 \frac{\pi(x-2y)}{a} + \cos^2 \frac{2\pi(x-y)}{a} + \cos^2 \frac{2\pi(x+y)}{a} \right], \quad (\text{S89})$$

whose profile in a single unit cell is plotted in Fig. S9(a). In practice, this potential can be generated by six standing-wave lasers with amplitude profiles given by

$$\cos \frac{2\pi[\cos \theta(2x \pm y)/\sqrt{3} + \sin \theta z]}{\lambda_{\text{al}}}, \quad \cos \frac{2\pi[\cos \theta(x \pm 2y)/\sqrt{3} + \sin \theta z]}{\lambda_{\text{al}}}, \quad \text{and} \quad \cos \frac{2\pi[\cos \theta'(x \pm y)/\sqrt{2} + \sin \theta' z]}{\lambda_{\text{al}}}, \quad (\text{S90})$$

where  $\theta = \arccos(\sqrt{3}\lambda_{\text{al}}/2a)$  and  $\theta' = \arccos(\sqrt{2}\lambda_{\text{al}}/a)$  are the tilt angles from the  $x$ - $y$  plane. Therefore, we can rather freely choose  $\lambda_{\text{al}}$  such that the auxiliary lattice only selectively traps a certain metastable state of atoms, such as the  $^3\text{P}_0$  state of alkaline-earth atoms. The on-site loss rate  $\kappa$  can be controlled by the strength of an additional laser that couples the metastable state to a certain unstable state, such as the  $^1\text{P}_1$  state of alkaline-earth atoms.

To overcome the difficulty (ii), we first note that the effective Rabi coupling  $\Omega_{\text{tb}}$  within the tight-binding approximation can be related to the spatial distribution of the Rabi coupling  $\Omega(\mathbf{r})$  via

$$\Omega_{\text{tb}} = \int d^2\mathbf{r} \Omega(\mathbf{r}) w_{\text{a}}^*(\mathbf{r} - \mathbf{r}_{\text{a}}) w_{\text{l}}(\mathbf{r} - \mathbf{r}_{\text{l}}), \quad (\text{S91})$$

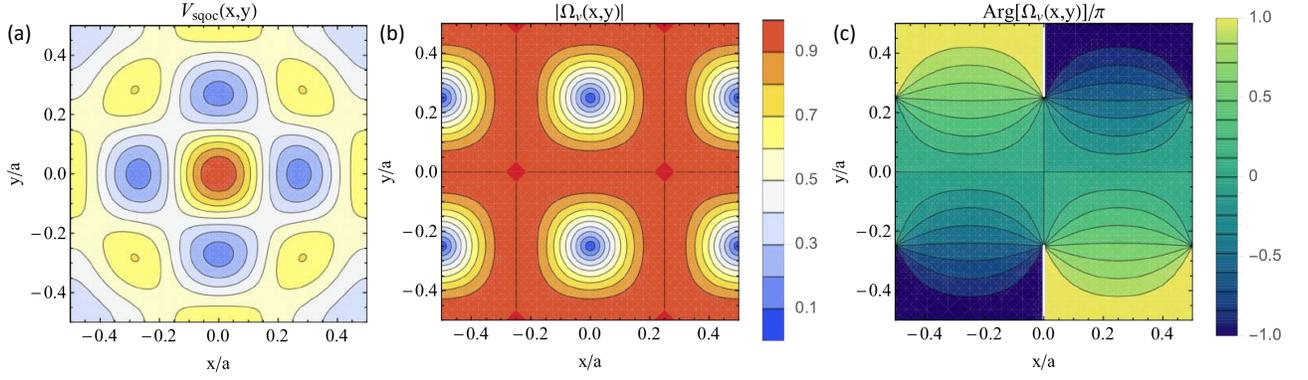


FIG. S9. (a) Square-octagon pattern of the auxiliary lattice potential  $V_{\text{sqoc}}(\mathbf{r})$  [see also Fig. S8(a)]. (b) Magnitude and (c) phase patterns of the vertical Rabi coupling  $\Omega_v(\mathbf{r})$  given in Eq. (S92). The units in (a) and (b) are set to be the largest  $V_{\text{sqoc}}(\mathbf{r})$  and  $|\Omega_v(\mathbf{r})|$ .

where  $\omega_1$  and  $\omega_a$  are the Wannier functions of the primary and auxiliary lattices, respectively. Therefore, the horizontal couplings  $a_2^\dagger(c_2 + ic_4)$  and  $a_1^\dagger(c_3 + ic_1)$  can easily be achieved by a running wave  $\Omega_h(\mathbf{r}) \propto \exp(i\frac{2\pi}{a}x)$  along the  $x$  direction, with the phase difference between  $c_2$  ( $c_3$ ) and  $c_4$  ( $c_1$ ) imprinted by the spatial phase variation of  $\Omega_h(\mathbf{r})$ . On the other hand, for the vertical couplings  $a_3^\dagger(c_2 + ic_3)$  and  $a_4^\dagger(c_1 + ic_4)$ , we cannot simply apply a running wave along the  $y$  direction; otherwise we will obtain  $a_4^\dagger(c_4 + ic_1)$  instead of  $a_4^\dagger(c_1 + ic_4)$ . To imprint the desired phase information, we can engineer the Rabi-frequency pattern to be

$$\Omega_v(\mathbf{r}) \propto \cos \frac{2\pi y}{a} - i \sin \frac{2\pi x}{a} \sin \frac{2\pi y}{a}, \quad (\text{S92})$$

which can be created by three standing wave lasers with amplitude profiles

$$\cos \frac{2\pi(\cos \alpha y + \sin \alpha z)}{\lambda_c} \text{ and } \cos \frac{2\pi[\cos \alpha'(x \pm y)/\sqrt{2} + \sin \alpha' z]}{\lambda_c}, \quad (\text{S93})$$

where  $\alpha = \arccos(\lambda_c/a)$  and  $\alpha' = \arccos(\sqrt{2}\lambda_c/a)$  are the tilt angles from the  $x$ - $y$  plane. We plot the spatial pattern of the magnitude and phase parts of  $\Omega_v$  [Eq. (S92)] in Figs. S9(b) and (c), where we can clearly find some vortices indicated by the zeros of  $|\Omega_v(\mathbf{r})|$  accompanied by phase windings. This observation is consistent with the existence of a  $\pi$  flux in the primary lattice.

## IX. NON-HERMITIAN SECOND-ORDER TOPOLOGICAL PHASES IN 3D

### A. Model

We consider a minimal model of a 3D non-Hermitian SOTI on a cubic lattice:

$$H_{3\text{D}}(\mathbf{k}) = [m + t(\cos k_x + \cos k_y + \cos k_z)]\tau_z + [(\Delta_1 \sin k_x + i\gamma_0)\sigma_x + (\Delta_1 \sin k_y + i\gamma_0)\sigma_y + (\Delta_1 \sin k_z + i\gamma_z)\sigma_z]\tau_x + \Delta_2(\cos k_x - \cos k_y)\tau_y, \quad (\text{S94})$$

where we have set the lattice constant  $a_0 = 1$ ,  $\sigma_i$  and  $\tau_i$  for  $i = x, y, z$  are Pauli matrices acting on spin and orbital/sublattice degrees of freedom, respectively, and  $m, t, \Delta_1, \Delta_2, \gamma_0$  and  $\gamma_z$  are real parameters. Note that the Hermitian part of  $H_{3\text{D}}(\mathbf{k})$  supports chiral hinge modes propagating along the  $z$  direction [20].

For  $\Delta_2 = 0$ , the Hermitian part of  $H_{3\text{D}}(\mathbf{k})$  is invariant under time reversal  $\mathcal{T} = \sigma_y \mathcal{K}$ , where  $\mathcal{K}$  being the complex conjugation operator,  $\mathcal{M}_x = i\sigma_x \tau_z$  is the  $x$  mirror reflection,  $\mathcal{M}_y = i\sigma_y \tau_z$  is the  $y$  mirror reflection, and  $C_4 = \exp(-i\pi\sigma_z/4)$  is the  $\pi/2$  rotation about the  $z$  axis. These symmetries are broken by both non-Hermitian terms including  $\gamma_0$  and terms including  $\Delta_2$ . However,  $H_{3\text{D}}(\mathbf{k})$  is invariant under the mirror-rotation symmetry operation  $\mathcal{M}_{xy} = C_4 \mathcal{M}_y$  with

$$\mathcal{M}_{xy} H_{3\text{D}}(k_x, k_y, k_z) \mathcal{M}_{xy}^{-1} = H_{3\text{D}}(k_y, k_x, k_z). \quad (\text{S95})$$

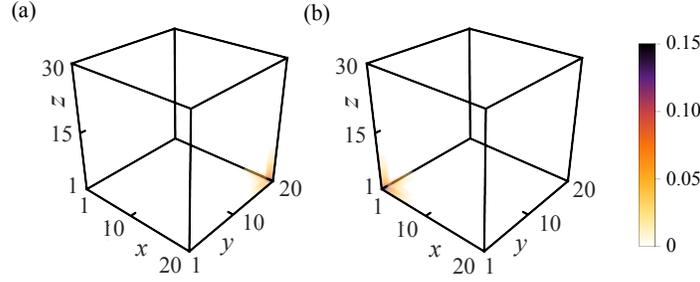


FIG. S10. Probability density distributions  $|\Phi_{n,R}|^2$  ( $n$  is the index of an eigenstate and  $R$  specifies a lattice site) of mid-gap modes for a 3D non-Hermitian SOTI with open boundaries along all the directions (a) for  $m = -2$  and  $\gamma_z = -0.2$ , and (b) for  $m = 2$  and  $\gamma_z = 0.2$ . The mid-gap states (with eigenenergy of 0.035) are only localized at one corner on the  $x = y$  plane. The number of unit cells is  $20 \times 20 \times 30$  with  $t = 1$ ,  $\gamma_0 = 0.7$ ,  $\Delta_1 = 1.2$ , and  $\Delta_2 = 1.2$ .

The bulk energy bands of the Hamiltonian  $H_{3D}(\mathbf{k})$  are obtained as

$$\begin{aligned} \bar{E}_{\pm}(\mathbf{k}) = & \pm \left[ -2\gamma_0^2 - \gamma_z^2 + (t \cos k_x + t \cos k_y + t \cos k_z + m)^2 + 2i\Delta_1 (\gamma_0 \sin k_x + \gamma_0 \sin k_y + \gamma_z \sin k_z) \right. \\ & \left. + \Delta_2^2 (\cos k_x - \cos k_y)^2 - \Delta_1^2 (\cos 2k_x + \cos 2k_y + \cos 2k_z - 3) / 2 \right]^{\frac{1}{2}}. \end{aligned} \quad (\text{S96})$$

where the upper and lower branches are two-fold degenerate, respectively. The Hamiltonian  $H_{3D}(\mathbf{k})$  is defective at the exceptional points (EPs) with

$$\bar{E}_{\pm}(\mathbf{k}_{EP}) = 0, \quad (\text{S97})$$

if one of the following conditions is satisfied:

(1) EPs appear when  $k_x = 0$  and  $k_y = 0$ , and then Eq. (S97) reduces to

$$(t \cos k_z + m + 2t)^2 - (\gamma_z - i\Delta_1 \sin k_z)^2 = 2\gamma_0^2. \quad (\text{S98})$$

(2) EPs appear when  $k_x = \pi$  and  $k_y = \pi$ , and then Eq. (S97) reduces to

$$(t \cos k_z + m - 2t)^2 - (\gamma_z - i\Delta_1 \sin k_z)^2 = 2\gamma_0^2. \quad (\text{S99})$$

(3) EPs appear when  $k_x = 0$  ( $\pi$ ) and  $k_y = \pi$  ( $0$ ), and then Eq. (S97) reduces to

$$4\Delta_2^2 + (t \cos k_z + m)^2 - (\gamma_z - i\Delta_1 \sin k_z)^2 = 2\gamma_0^2. \quad (\text{S100})$$

(4) EPs appear when  $k_x = -k_y$  with  $k_y \neq 0$  and  $k_y \neq \pi$ , and then Eq. (S97) reduces to

$$(2t \cos k_y + t \cos k_z + m)^2 - \Delta_1^2 (\cos 2k_y + \cos 2k_z / 2 - 3/2) - \gamma_z^2 + 2i\gamma_z \Delta_1 \sin k_z = 2\gamma_0^2. \quad (\text{S101})$$

### B. Localization of second-order boundary states at one corner

As shown in the main text, the mid-gap states in the 3D non-Hermitian SOTI are localized at the right corner of the  $x = y$  plane [see Fig. 5(e) in the main text and Fig. S10(a)]. We note that the mid-gap states can also be localized at the left corner on the  $x = y$  plane when an opposite sign of the parameter  $m$  is considered, as shown in Fig. S10(b). The localization of the mid-gap states at one corner on the  $x = y$  plane results from the interplay between mirror-rotation symmetry  $\mathcal{M}_{xy}$  and non-Hermiticity.

### C. Effect of a different type of asymmetric hopping and non-Hermiticity on the localization of boundary states

In the 2D model, we have considered the effect of a different type of asymmetric hopping and non-Hermiticity (i.e., balanced gain and loss) on the localization of corner states in Sec. V. In this section, we study effect of a different type of asymmetric

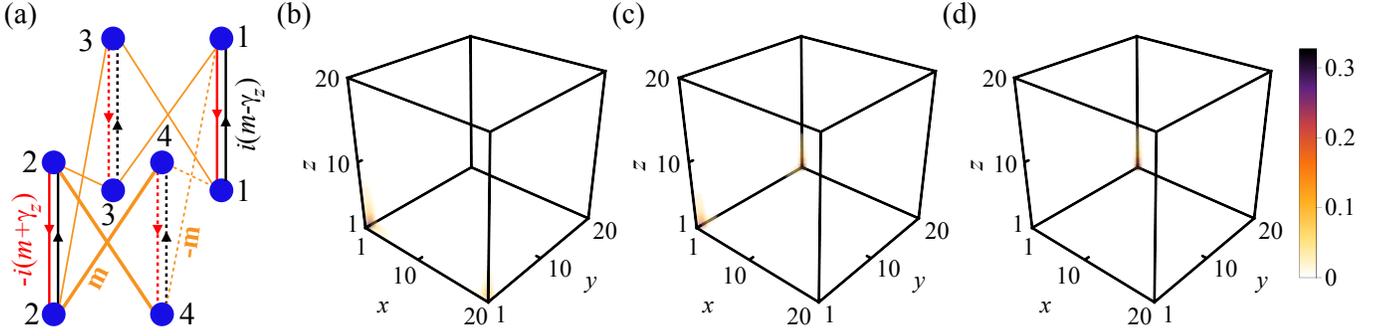


FIG. S11. (a) Real-space representation of the 3D model in Eq. (S102), which shows the particle hopping along the  $z$  direction between 2D layers. This 3D lattice is constructed by stacking the 2D lattice layer shown in Fig. S6(a). Along the  $z$  direction, the nearest and next-to-nearest neighbor hoppings are considered. The dashed lines indicate hopping terms with a negative sign. Probability density distributions  $|\Phi_{n,R}|^2$  ( $n$  is the index of an eigenstate and  $R$  specifies a lattice site) of mid-gap modes with open boundaries along all the directions: (b) for  $\gamma_x = 0$  and  $\gamma_y = 0.5$ , (c) for  $\gamma_x = 0.5$  and  $\gamma_y = 0$ , and (d) for  $\gamma_x = 0.5$  and  $\gamma_y = -0.5$ . The mid-gap states (with eigenenergy of 0.04) are localized at more than one corner for  $\gamma_x = 0$  or  $\gamma_y = 0$ . The number of unit cells is  $20 \times 20 \times 20$  with  $\gamma_z = -0.2$ ,  $m = -1$ ,  $t_x = t_y = 1.0$  and  $\lambda = 1.5$ .

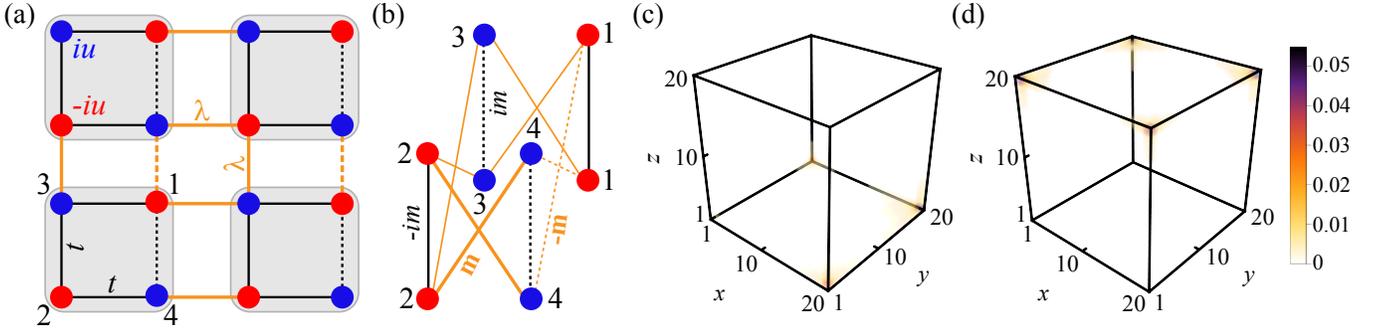


FIG. S12. (a,b) Real-space representation of the 3D model in Eq. (S103). The particle hopping in the  $(x, y)$ -plane, with the alternating on-site gain and loss (with the imaginary staggered potentials  $iu$  and  $-iu$ ) within each unit cell, is shown in (a). The particle hopping along the  $z$  direction between 2D layers is indicated in (b). This 3D lattice is constructed by stacking the 2D lattice layer shown in (a). The dashed lines indicate hopping terms with a negative sign. Probability density distributions  $|\Phi_{n,R}|^2$  ( $n$  is the index of an eigenstate and  $R$  specifies a lattice site) of mid-gap modes with open boundaries along all the directions: (c) for  $u = -0.2$ , and (d) for  $u = 0.2$ . The mid-gap states (with eigenenergy of 0.04) are localized at more than one corner. The number of unit cells is  $20 \times 20 \times 20$  with  $m = -1$ ,  $t = 1.0$  and  $\lambda = 1.5$ .

hopping and non-Hermiticity on the localization of second-order boundary modes in 3D non-Hermitian SOTIs. The non-Hermitian terms of the 3D model studied in our manuscript take the form of an imaginary Zeeman field [10, 21]. Therefore, to investigate the effect of a different type of asymmetric hopping on the localization of second-order boundary modes in 3D SOTIs, we consider a 3D non-reciprocal lattice model by stacking the 2D lattice layers as shown in Fig. S6(a). The particle hoppings along the  $z$  direction between 2D layers are indicated in Fig. S11(a). In momentum space, the Hamiltonian has the form

$$\begin{aligned} \bar{H}_{3D}(\mathbf{k}) = & [t_x + \lambda \cos(k_x)] \tau_x - [\lambda \sin(k_x) + i\gamma_x] \tau_y \sigma_z + [t_y + \lambda \cos(k_y)] \tau_y \sigma_y + [\lambda \sin(k_y) + i\gamma_y] \tau_y \sigma_x \\ & + m \cos(k_z) (\tau_x + \tau_y \sigma_y) + [m \sin(k_z) - i\gamma_z \cos(k_z)] \tau_z, \end{aligned} \quad (\text{S102})$$

where the Hermitian part of the Hamiltonian  $\bar{H}_{3D}(\mathbf{k})$  supports four-degenerate chiral hinge modes propagating along the  $z$  direction. Note that 3D Hermitian SOTIs can be present even in the absence of crystalline symmetries, as in the 2D case [7].

When the larger hopping strength with amplitude  $-i(m + \gamma_z)$  (i.e.,  $m$  and  $\gamma_z$  have the same signs) along the  $z$  direction is considered [see Fig. S11(a)], the second-order boundary modes are localized at corners of the bottom side (i.e.,  $z = 1$  plane), as shown in Figs. S11(b-d). In this case, for the larger hopping amplitude with  $(t_y + \gamma_y)$  along the  $y$  direction and the symmetric hopping along the  $x$  direction, the second-order boundary states are localized at both the lower-left and lower-right corners of  $z = 1$  plane [see Fig. S11(b)]. In contrast, these second-order boundary modes are localized at both the lower-left and upper-left corners for the larger hopping amplitude with  $(t_x + \gamma_x)$  along the  $x$  direction and the symmetric hopping along the  $y$  direction [see Fig. S11(c)]. Moreover, the asymmetric hoppings along both the  $x$  and  $y$  directions make the second-order boundary modes localized at one corner [see Fig. S11(d)]. Therefore, the localization of the second-order boundary modes in

the 3D non-reciprocal lattice model also depends on the type of asymmetric hopping.

In addition to the different type of asymmetric hopping, the second-order boundary modes in 3D systems can be localized at more than one corner in the presence of a different type of non-Hermiticity i.e., balanced gain and loss. As shown in Figs. S12(a) and (b), we consider the alternating on-site gain and loss with symmetric particle hopping, where the imaginary staggered potentials are indicated by  $iu$  and  $-iu$ . The Bloch Hamiltonian is written as

$$\begin{aligned} \tilde{H}_{3D}(\mathbf{k}) = & [t + \lambda \cos(k_x)] \tau_x - \lambda \sin(k_x) \tau_y \sigma_z + [t + \lambda \cos(k_y)] \tau_y \sigma_y + \lambda \sin(k_y) \tau_y \sigma_x \\ & + m \cos(k_z) (\tau_x + \tau_y \sigma_y) + m \sin(k_z) \tau_z - iu \tau_z. \end{aligned} \quad (\text{S103})$$

Figures S12(c) and (d) show the probability density distributions for  $u = -0.2$  and  $u = 0.2$ , respectively. In the presence of the balanced gain and loss, the second-order boundary modes are localized at more than one corner of either the top or the bottom side in 3D systems.

#### D. Low-energy effective Hamiltonians

The localization of the mid-gap states at one corner on the  $x = y$  plane results from the symmetry  $\mathcal{M}_{xy}$  and non-Hermiticity, and each mid-gap mode is a mutual topological state of two intersecting surfaces parallel to the  $z$ -axis. In this section, we present low-energy effective Hamiltonians to explain this effect. We label the four surfaces of a cubic sample as I, II, III, and IV (see Fig. S13). For the sake of simplicity, we consider the case of  $\min\{-m, t, \Delta_1, \Delta_2\} > 0$ . In this case, the low-energy bands of the Hermitian part of  $H_{3D}(\mathbf{k})$  lie around the  $\Gamma$  point of the Brillouin zone. Therefore, we consider a continuum model of the lattice Hamiltonian [see Eq. (S94)] by expanding its wavevector  $\mathbf{k}$  to second order around the  $\Gamma = (0, 0, 0)$  point of the Brillouin zone, obtaining

$$\begin{aligned} \bar{H}_{\text{cm}}(\mathbf{k}) = & \left[ m + 3t - \frac{t}{2} (k_x^2 + k_y^2 + k_z^2) \right] \tau_z + [(\Delta_1 k_x + i\gamma_0) \sigma_x + (\Delta_1 k_y + i\gamma_0) \sigma_y + (\Delta_1 k_z + i\gamma_z) \sigma_z] \tau_x \\ & + \frac{\Delta_2}{2} (k_y^2 - k_x^2) \tau_y. \end{aligned} \quad (\text{S104})$$

We first investigate the surface I. By expressing  $k_y$  as  $-i\partial_y$ , we can rewrite the Hamiltonian  $\bar{H}_{\text{cm}}(\mathbf{k})$  as  $\bar{H}_{\text{cm}}(k_x, -i\partial_y, k_z) = \tilde{H}_{\text{cm},1}(k_x, -i\partial_y, k_z) + \tilde{H}_{\text{cm},2}(k_x, -i\partial_y, k_z)$ , where

$$\tilde{H}_{\text{cm},1}(k_x, -i\partial_y, k_z) = \left( m + 3t + \frac{t}{2} \partial_y^2 \right) \tau_z - i\Delta_1 \partial_y \sigma_y \tau_x \quad (\text{S105})$$

is Hermitian, and

$$\tilde{H}_{\text{cm},2}(k_x, -i\partial_y, k_z) = \Delta_1 (k_x \sigma_x + k_z \sigma_z) \tau_x + i\gamma_0 (\sigma_x + \sigma_y) \tau_x + i\gamma_z \sigma_z \tau_x - \frac{\Delta_2}{2} \tau_y \partial_y^2 \quad (\text{S106})$$

is treated as a perturbation for  $\max\{\Delta_2, |\gamma_0|, |\gamma_z|\} \ll \max\{|m + 3t|, t/2, \Delta_1\}$ . Note that we have neglected insignificant terms  $k_x^2$  and  $k_z^2$  for  $\mathbf{k}$  around the  $\Gamma$  point.

To obtain the eigenvalue equation  $\tilde{H}_{\text{cm},1}\phi_1(y) = E\phi_1(y)$ , with  $E = 0$  subject to the boundary condition  $\phi_1(0) = \phi_1(+\infty) = 0$ , we write the solution in the following form:

$$\phi_1(y) = \mathcal{N}_y \sin(\alpha y) e^{-\beta y} e^{i(k_x x + k_z z)} \chi_1, \quad \text{Re}(\beta) > 0, \quad (\text{S107})$$

where the normalization constant is given by  $\mathcal{N}_y = 2\sqrt{\beta(\alpha^2 + \beta^2)}/\alpha^2$ , and the eigenvector  $\chi_1$  satisfies  $\sigma_y \tau_y \chi_1 = \chi_1$ . Then the effective Hamiltonian for the surface I can be obtained in this basis as

$$\mathcal{H}_{\text{surf}}^I = \int_0^{+\infty} \phi_1^*(y) \tilde{H}_{\text{cm},2} \phi_1(y) dy. \quad (\text{S108})$$

Therefore, we have

$$\mathcal{H}_{\text{surf}}^I = \Delta_2 \left( 3 + \frac{m}{t} \right) \varrho_z - (\Delta_1 k_x + i\gamma_0) \varrho_x - (\Delta_1 k_z + i\gamma_z) \varrho_y. \quad (\text{S109})$$

The low-energy effective Hamiltonians for the surfaces II, III and IV can be obtained by the same procedures

$$\mathcal{H}_{\text{surf}}^{\text{II}} = \Delta_2 \left( 3 + \frac{m}{t} \right) \varrho_z + (\Delta_1 k_y + i\gamma_0) \varrho_x + (\Delta_1 k_z + i\gamma_z) \varrho_y, \quad (\text{S110})$$

$$\mathcal{H}_{\text{surf}}^{\text{III}} = \Delta_2 \left( 3 + \frac{m}{t} \right) \varrho_z + (\Delta_1 k_x + i\gamma_0) \varrho_x - (\Delta_1 k_z + i\gamma_z) \varrho_y, \quad (\text{S111})$$

$$\mathcal{H}_{\text{surf}}^{\text{IV}} = \Delta_2 \left( 3 + \frac{m}{t} \right) \varrho_z - (\Delta_1 k_y + i\gamma_0) \varrho_x + (\Delta_1 k_z + i\gamma_z) \varrho_y, \quad (\text{S112})$$

for  $3 + m/t > 0$ .

For the Hermitian case (i.e.,  $\gamma_0 = 0$ ), the last two kinetic terms of the effective Hamiltonian in Eqs. (S109)-(S112) describe the gapless surface states, which are gapped out by the first terms with the Dirac mass. To derive the second-order boundary modes, we introduce a new coordinate  $p$  along anticlockwise direction within the planes parallel to the  $xy$  plane, and we rewrite Eqs. (S109)-(S112) as

$$\mathcal{H}_{\text{surf}} = \Delta_2 \left( 3 + \frac{m}{t} \right) \varrho_z - [-i\Delta(p)\partial p + i\gamma(p)] \varrho_x - (\Delta_1 k_z + i\gamma_z) \varrho_y, \quad (\text{S113})$$

where  $\Delta(p) = \Delta_1, -\Delta_1, \Delta_1, -\Delta_1$ , and  $\gamma(p) = \gamma_0, -\gamma_0, -\gamma_0, \gamma_0$  along the anticlockwise direction of the four surfaces. According to Eq. (S113), it is easy to verify that the Hermitian part (i.e.,  $\gamma_0 = 0$ ) of  $H_{3\text{D}}(\mathbf{k})$  supports four-fold degenerate gapless hinge modes for  $k_z = 0$  (analogous to the Jackiw-Rebbi model [22]).

In the presence of non-Hermiticity, we first solve the boundary mode along the hinge intersected by the surfaces I and II. We write this boundary mode in the following form:

$$\Psi_h^{\text{I}} = e^{ik_z z + \kappa_{\text{I},1} \tilde{p}} \chi_{h,1}, \quad \text{Re}(\kappa_{\text{I},1}) > 0, \quad \tilde{p} = p - L < 0, \quad (\text{S114})$$

$$\Psi_h^{\text{II}} = e^{ik_z z + \kappa_{\text{II},1} \tilde{p}} \chi_{h,1}, \quad \text{Re}(\kappa_{\text{II},1}) < 0, \quad \tilde{p} = p - L > 0, \quad (\text{S115})$$

where  $L$  is the width of cubic sample, and  $\chi_{h,1}$  is the eigenvector. To find the gapless boundary mode along the hinge intersected by the surfaces I and II, the following equations are satisfied:

$$\kappa_{\text{I},1} = \frac{\gamma_0 \pm \sqrt{\delta^2 + (\Delta_1 k_z + i\gamma_z)^2}}{\Delta_1}, \quad \kappa_{\text{II},1} = \frac{\gamma_0 \pm \sqrt{\delta^2 + (\Delta_1 k_z + i\gamma_z)^2}}{\Delta_1}, \quad \text{Re}(\kappa_{\text{I},1}) > 0, \quad \text{Re}(\kappa_{\text{II},1}) < 0, \quad (\text{S116})$$

where  $\delta = \Delta_2 (3 + m/t)$ .

By applying the same procedures, to have the zero gapless boundary modes along hinges intersected by surfaces II and III, surfaces III and IV and surfaces IV and I, we have the following equalities:

$$\kappa_{\text{II},2} = \frac{\gamma_0 \pm \sqrt{\delta^2 + (\Delta_1 k_z + i\gamma_z)^2}}{\Delta_1}, \quad \kappa_{\text{III},2} = \frac{-\gamma_0 \pm \sqrt{\delta^2 + (\Delta_1 k_z + i\gamma_z)^2}}{\Delta_1}, \quad \text{Re}(\kappa_{\text{II},2}) > 0, \quad \text{Re}(\kappa_{\text{III},2}) < 0, \quad (\text{S117})$$

$$\kappa_{\text{III},3} = \frac{-\gamma_0 \pm \sqrt{\delta^2 + (\Delta_1 k_z + i\gamma_z)^2}}{\Delta_1}, \quad \kappa_{\text{IV},3} = \frac{-\gamma_0 \pm \sqrt{\delta^2 + (\Delta_1 k_z + i\gamma_z)^2}}{\Delta_1}, \quad \text{Re}(\kappa_{\text{III},3}) > 0, \quad \text{Re}(\kappa_{\text{IV},3}) < 0, \quad (\text{S118})$$

$$\kappa_{\text{IV},4} = \frac{-\gamma_0 \pm \sqrt{\delta^2 + (\Delta_1 k_z + i\gamma_z)^2}}{\Delta_1}, \quad \kappa_{\text{I},4} = \frac{\gamma_0 \pm \sqrt{\delta^2 + (\Delta_1 k_z + i\gamma_z)^2}}{\Delta_1}, \quad \text{Re}(\kappa_{\text{IV},4}) > 0, \quad \text{Re}(\kappa_{\text{I},4}) < 0. \quad (\text{S119})$$

According to Eqs. (S116)-(S119), it is straightforward to verify that the gapless boundary modes, under the periodic boundary condition along the  $z$  direction, appear only along the hinge intersected by the surfaces II and III if  $|\gamma_0| > \sqrt{\delta^2 - \gamma_z^2}$  with  $|\delta| > |\gamma_z|$  or  $|\gamma_z| > |\delta|$ . In summary, the simple low-energy effective Hamiltonian presented here can explain the existence and the localization at one hinge of second-order gapless boundary modes due to the interplay between mirror-rotation symmetry and non-Hermiticity.

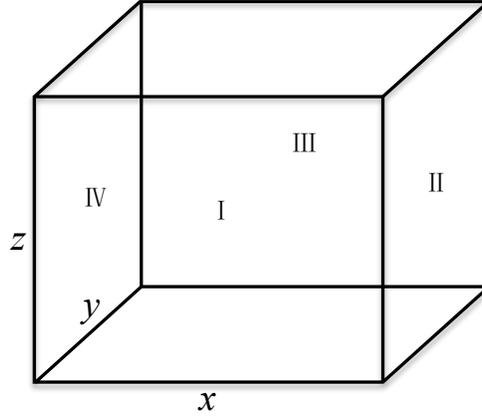


FIG. S13. Schematic illustration of a 3D non-Hermitian SOTI in a cubic sample. I, II, III and IV label the four surfaces of the lattice.

### E. Topological index

As shown in the main text, due to mirror-rotation symmetry  $\mathcal{M}_{xy}$ , we can write the Hamiltonian  $H_{3D}(\mathbf{k})$  into the block-diagonal form with  $k_x = k_y = k$  as

$$\tilde{U}^{-1} H_{3D}(\mathbf{k}) \tilde{U} = \begin{bmatrix} H_+(k, k_z) & 0 \\ 0 & H_-(k, k_z) \end{bmatrix}, \quad (\text{S120})$$

where  $H_+(k, k_z)$  acts on the  $+i$  mirror-rotation subspace, and  $H_-(k, k_z)$  acts on the  $-i$  mirror-rotation subspace. The unitary transformation  $\tilde{U}$  is

$$\tilde{U} = \begin{bmatrix} 0 & -\frac{1+i}{2} & 0 & \frac{1+i}{2} \\ \frac{1+i}{2} & 0 & -\frac{1+i}{2} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \end{bmatrix}, \quad (\text{S121})$$

and  $H_+(k, k_z)$  and  $H_-(k, k_z)$  are

$$H_+(k, k_z) = -[m + 2t \cos(k) + t \cos(k_z)] \sigma_z + \sqrt{2} [\Delta_1 \sin(k) + i\gamma_0] \sigma_y - [\Delta_1 \sin(k_z) + i\gamma_z] \sigma_x, \quad (\text{S122})$$

$$H_-(k, k_z) = -[m + 2t \cos(k) + t \cos(k_z)] \sigma_z - \sqrt{2} [\Delta_1 \sin(k) + i\gamma_0] \sigma_y - [\Delta_1 \sin(k_z) + i\gamma_z] \sigma_x. \quad (\text{S123})$$

To account for the non-Bloch-wave behavior of the non-Hermitian systems and to capture the essential physics with analytical results, we consider a low-energy continuum mode of  $H_{3D}(\mathbf{k})$  and  $H_{\pm}(k, k_z)$ . Then the non-Bloch-wave behavior can be taken into account by replacing the real wavevector  $k$  in Eqs. (S120)-(S123) with the complex one after applying the degenerate perturbation theory to Hamiltonian  $H_{3D}$  with open boundaries along the  $x$ ,  $y$  and  $z$  directions for  $\min\{|m + 3t|, |t|, |\Delta_1|\} \gg \max\{|\gamma_0|, |\gamma_z|\}$  [10]:

$$k \rightarrow k + ik', \quad k_z \rightarrow k_z + ik'_z, \quad (\text{S124})$$

with

$$k' = -\frac{\gamma_0}{\Delta_1}, \quad k'_z = -\frac{\gamma_z}{\Delta_1}. \quad (\text{S125})$$

Then, we rewrite Eq. (S122) and (S123) as

$$\bar{H}_+(k, k_z) = - \left[ m + 3t - t \left( k - i \frac{\gamma_0}{\Delta_1} \right)^2 - \frac{t}{2} k_z^2 \right] \sigma_z + \sqrt{2} \left[ \Delta_1 \left( k - i \frac{\gamma_0}{\Delta_1} \right) + i\gamma_0 \right] \sigma_y - \left[ \Delta_1 \left( k_z - i \frac{\gamma_z}{\Delta_1} \right) + i\gamma_z \right] \sigma_x, \quad (\text{S126})$$

$$\bar{H}_-(k, k_z) = - \left[ m + 3t - t \left( k - i \frac{\gamma_0}{\Delta_1} \right)^2 - \frac{t}{2} k_z^2 \right] \sigma_z - \sqrt{2} \left[ \Delta_1 \left( k - i \frac{\gamma_0}{\Delta_1} \right) + i\gamma_0 \right] \sigma_y - \left[ \Delta_1 \left( k_z - i \frac{\gamma_z}{\Delta_1} \right) + i\gamma_z \right] \sigma_x. \quad (\text{S127})$$

The Chern numbers  $C_+$  and  $C_-$ , corresponding to the  $\bar{H}_+(k, k_z)$  and  $\bar{H}_-(k, k_z)$ , are defined as

$$C_{\pm} = \frac{1}{2\pi} \int_{\text{BZ}} F_{\pm}(k, k_z) dk dk_z, \quad (\text{S128})$$

where  $F_{\pm}(k, k_z)$  is the Berry curvature

$$F_{\pm}(k, k_z) = \partial_k A_{\pm}^{k_z}(k, k_z) - \partial_{k_z} A_{\pm}^k(k, k_z), \quad (\text{S129})$$

and  $A_{\pm}^{\mu}$  is the Berry connection

$$A_{\pm}^{\mu}(k, k_z) = i \langle \chi_{\pm}(k, k_z) | \partial_{\mu} \phi_{\pm}(k, k_z) \rangle, \quad (\text{S130})$$

where  $|\phi_{\pm}^{\alpha}(\mathbf{k})\rangle$  and  $|\chi_{\pm}^{\alpha}(\mathbf{k})\rangle$  are the right and left eigenstates of  $\bar{H}_{\pm}(k, k_z)$ . Then, the total Chern number is given by

$$C = C_+ - C_-. \quad (\text{S131})$$

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