Bulk-Boundary Correspondence in Non-Hermitian Systems

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Bulk-boundary correspondence is fundamental and important in topological physics; however, it is invalid in certain non-Hermitian systems. Here we report that the way of non-Hermiticity appearance may alter the system topology, induce a topological phase transition, and invalidate the bulk-boundary correspondence if non-Hermiticity breaks the chiral-inversion symmetry of the system. Alternatively introducing non-Hermiticity without breaking the chiral-inversion symmetry, the bulk-boundary correspondence recovers with all the bulk states being extended and the non-Hermitian skin effect vanishes. The vorticity of topological defects in the vector field that associated with the Bloch Hamiltonian is a topological invariant, the change of which predicts the (non)existence of edge states. Our findings reveal the roles played by symmetry and non-Hermiticity, and provide insights into the non-Hermitian topological phases of matter.

**Introduction.**—Topological theory has been well established in condensed matter physics \cite{[130]81} and recent experimental progresses in optics boost the development of topological photonics \cite{[32]39}. The existence of gapless edge states of a system under open boundary condition (OBC) is predictable from the change of topological invariants associated with the bulk topology of system under periodical boundary condition (PBC), known as the (conventional) bulk-boundary correspondence, which is ubiquitously applicable in Hermitian systems.

In parallel, non-Hermitian physics exhibits considerable intriguing features \cite{[10]73}: the unexpected novel interface states appear between non-Hermitian periodic media with distinct topologies \cite{[74]87}. These stimulate the studies of topological phases and edge states in non-Hermitian systems \cite{[88]116}. Employing the left and right eigenstates \cite{[46]50}, non-Hermitian band theory and the topological characterization are developed; the Chern number, generalized Berry phase and winding numbers are quantized as topological invariants \cite{[118]126}.

Remarkably, the bulk-boundary correspondence is invalid in certain non-Hermitian topological systems \cite{[117]118}: The systems under PBC and OBC have dramatically different energy spectra, and all the eigenstates localize near system boundaries (the non-Hermitian skin effect) \cite{[119]120}. These have received great research interests in non-Hermitian systems of asymmetric Su-Schrieffer-Heeger (SSH) model, topological insulators, and nodal-line semimetals \cite{[119]125}. To predict the (non)existence of edge states, the biorthogonal bulk-boundary correspondence is established using a coined biorthogonal polarization \cite{[119]120}; alternatively, a non-Bloch topological invariant defined on the generalized Brillouin zone is suggested as the non-Bloch bulk-boundary correspondence \cite{[120]19}. In contrast, the non-Hermiticity does not inevitably destroy the bulk-boundary correspondence \cite{[117]118, [75]76, [91]95}, and its validity is verified in a $\mathcal{PT}$-symmetric non-Hermitian extension of SSH model with staggered couplings and losses \cite{[88]116, [90]}. The existence of topologically protected states at the interface of media with distinct topologies is predicted from the bulk topology, characterized by a geometric phase related winding number \cite{[87]89}. However, why bulk-boundary correspondence fails in certain non-Hermitian systems but remains valid in some other non-Hermitian systems? What role the non-Hermiticity plays in the breakdown of bulk-boundary correspondence and the appearance of non-Hermitian skin effect? Whether symmetry protects non-Hermitian topological phases and how to characterize the topological properties?

In this Letter, we report that symmetry plays an important role for the validity of bulk-boundary correspondence in non-Hermitian systems and non-Hermiticity may alter the system topology. We elucidate that the breakdown of bulk-boundary correspondence in non-Hermitian systems attributes to the absence of chiral-inversion symmetry in the presence of non-Hermiticity, the introducing of which directly induces a topological phase transition and the non-Hermitian skin effect. Fixing the chiral-inversion symmetry through alternatively introducing the non-Hermiticity, the energy spectrum under OBC is not altered; remarkably, the bulk-boundary correspondence recovers. The band touching degeneracy (exceptional) points are topological defects with vortex or antivortex in a vector field associated with the Bloch Hamiltonian, and the vorticity is a topological invariant. The change of vorticity correctly predicts the (non)existence of topological edge states.

**Non-Hermitian system.**—We first consider a non-Hermitian SSH model as depicted in Fig. 1(a) \cite{[120]19}. Under PBC, the topological system is translational symmetric, the Bloch Hamiltonian is

$$H_a(k) = (t_1 + t_2 \cos k) \sigma_x + (t_2 \sin k - i \gamma) \sigma_y,$$

where $\gamma$ is the peak-to-peak alternating current, and $t_1$, $t_2$, and $\gamma$ are the hopping parameters, respectively.

**FIG. 1.** (a, b) Schematic of the dimerized SSH lattices, $H_a, b \ [H_{a,b}(k)]$ is the Hamiltonian in the real-space ($k$-space). The intra cell couplings are $\mu = t_1 - \gamma$ and $\nu = t_1 + \gamma$. The existence of topologically protected states at the interface of media with distinct topologies is predicted from the bulk topology, characterized by a geometric phase related winding number $\text{\Semi}[87][89]$. However, why bulk-boundary correspondence fails in certain non-Hermitian systems but remains valid in some other non-Hermitian systems? What role the non-Hermiticity plays in the breakdown of bulk-boundary correspondence and the appearance of non-Hermitian skin effect? Whether symmetry protects non-Hermitian topological phases and how to characterize the topological properties?
where $\sigma_{x,y}$ are the Pauli matrices. The intercell coupling is $t_2$. Set $\mu = t_1 - \gamma$ and $\nu = t_1 + \gamma$ for convenience, the asymmetric intracell coupling strength ($\mu \neq \nu^*$) raises the non-Hermiticity. System $a$ has the chiral symmetry. The eigenvalues are symmetric $E_{a,\pm} = \pm \sqrt{t_1^2 + \mu \nu + t_2 (\mu e^{i \theta} + \nu e^{-i \theta})}$ [Fig. 2(a)]. The wave vector is $k = \pi n / N$, $m \in [1, 2n]$ ($m, n$ are positive integers) for the discrete lattice size $N = 4n$.

Topological phase transition induced by symmetry breaking.—In Hermitian case ($\gamma = 0$), system $a$ is chiral-inversion symmetric that

$$(SP) H_a(k) (SP)^{-1} = -H_a(-k), U_{SP} H_a U_{SP}^{-1} = -H_a.$$  \tag{2}

The constrains are for a combined chiral-inversion symmetry and the operators $SP$ and $U_{SP}$ are unitary. Notably, two band touching degeneracy points exist under PBC [Fig 2(d)], and the eigenstates are symmetric or antisymmetric. However, if non-Hermitian asymmetry and the operators $SP$, combined the constrains are for a unitary, two band touching degeneracy points exist under PBC [Fig 2(d)] under OBC with one intercell coupling $t_2$ missing, and (d) $H_a$ and $H_b$ under PBC at $\gamma = 0$. The band touching exceptional (degeneracy) points are indicated by the cyan (green) hollow circles. The system parameters are $N = 40$, $t_2 = 1$, and $\gamma = 1/2$ in (a-c).

The presence of non-Hermiticity directly induces a topological phase transition. The eigenstates under OBC are no longer symmetric/antisymmetric and the non-Hermitian skin effect occurs without symmetry protection, all the eigenstates are localized. This is reflected from the inverse participation ratio (IPR) $\sum_j |\psi_j|^4$ (each eigenstate is normalized to unity $\sum_j |\psi_j|^2 = 1$). IPR for the eigenstates of system $a$ (blue circles) is system size insensitive compared with IPR of system $b$ (black crosses) in Fig. 3(a).

The chiral-inversion symmetry holds when non-Hermiticity is alternatively introduced in system $b$ [Fig. 1(b)], where $SP = \sigma_x \otimes \sigma_y$ and $U_{SP} = P_{2n} \otimes I$ in Eq. (2), $\otimes$ is the Kronecker product, and $P_{2n}$ is a 90 degrees rotation of the $2n \times 2n$ identical matrix $I_{2n}$. Under symmetry protection, introducing non-Hermiticity does not directly induce a topological phase transition, and two degeneracy points can move in the parameter space without splitting into EP pairs [Figs. 2(b) and 2(d)]. The eigenstates under OBC are symmetric or antisymmetric. Figure 3(b) depicts the averaged IPR for the bulk eigenstates of system $b$, which is inversely proportional to the system size. This indicates that all the bulk states are extended and the non-Hermitian skin effect vanishes, even in regions that most bulk states are complex.

Systems $a$ and $b$ under OBC possess identical energy spectra as depicted in Fig. 2(c) [144], but with significantly different eigenstates: All the eigenstates of system $a$ localize near system boundary; in contrast, all the bulk states in system $b$ are extended, and only the edge states

![FIG. 2. Energy spectra for (a) (b) $H_a$ (H_b) under PBC, (c) $H_a$ and $H_b$ under OBC with one intercell coupling $t_2$ missing, and (d) $H_a$ and $H_b$ under PBC at $\gamma = 0$. The band touching exceptional (degeneracy) points are indicated by the cyan (green) hollow circles. The system parameters are $N = 40$, $t_2 = 1$, and $\gamma = 1/2$ in (a-c).](image)

![FIG. 3. (a) IPR of all the eigenstates, the blue circles (black crosses) are for system $a$ (b). (b) Averaged IPR for all the bulk states of system $b$, which scales as $1/N$. The system parameters are $t_1 = 1/4$, $\gamma = 1/2$, and $t_2 = 1$.](image)
localize near system boundary (Fig. 3). These reflect the distinct topologies of systems a and b, and manifest that the way of non-Hermiticity appearance affects the system topology. Notably, the non-Hermiticity solely induces nontrivial topology at $t_1 = t_2$.

Bulk-boundary correspondence.—The bulk-boundary correspondence recovers in both the regions with entirely real spectra and with complex spectra [Figs. 2(b) and 2(c)]. The recovery of bulk-boundary correspondence enables predicting the (non)existence of topologically protected edge states from the bulk topology of system b, the Bloch Hamiltonian of which has a four-site unit cell

$$H_b(k) = \begin{pmatrix}
0 & \mu & 0 & t_2 e^{-ik} \\
\nu & 0 & t_2 & 0 \\
t_2 & 0 & \nu & 0 \\
t_2 e^{ik} & 0 & \mu & 0
\end{pmatrix}.$$  \hspace{1cm} (3)

The eigenvalues $E_{b,\pm,\pm} = \pm \sqrt{t_2^2 + \mu \nu \pm 2t_2 \sqrt{\mu \nu} \cos(k/2)}$ ($k = 2\pi m/n, m \in [1, n]$) are symmetric. Through a similar transformation $U_{b,\mu} = \text{diag}(\sqrt{\mu}, \sqrt{\mu}, \sqrt{\nu}, \sqrt{\nu})$ with only nonzero diagonal elements, we obtain an equivalent Bloch Hamiltonian $U_{b,\mu} H_b(k) U_{b,\mu}^{-1}$, which is for system a with all the asymmetric intracell couplings substituted by the symmetric couplings $\sqrt{\mu \nu}$ and taken two unit cells as a compound one [74]. This equivalent system has a two-site unit cell and the Bloch Hamiltonian is $h_0(k) = (\sqrt{\mu \nu} + t_{2b} \cos k) \sigma_x + (t_{2b} \sin k) \sigma_y$, the eigenvalues are $E_{b,\pm} = \pm \sqrt{t_2^2 + \mu \nu + 2t_2 \sqrt{\mu \nu} \cos(k)}$ ($k = \pi m/n)$, $m \in [1, 2n]$), being identical with the eigenvalues of system b. The bulk topology of $h_0(k)$ correctly predicts the (non)existence of edge states in both systems a and b under OBC because they possess identical energy spectra [74]. Notably, $h_0(k)$ is identical with that alternatively found in Ref. 120 through solving $H_a$ under OBC.

For $\gamma = |r| e^{i\theta}$ ($-\pi \leq \theta \leq \pi$), the band gap closes at

$$(t_1^2 - |\gamma|^2)^2 + 4t_1^2 |\gamma|^2 \sin^2 \theta = t_1^4,$$  \hspace{1cm} (4)

and $\cos^2(k) = (t_1^2 + t_2^2 - |\gamma|^2 \cos(2\theta))/2t_1^2$. For real $\mu$ and $\nu$ at $\theta = 0$, the band touching points are degeneracy (exceptional) points at $t_1^2 = +(-) t_1^2 + \gamma^2$ [119] [120], being topological defects carrying integer (half-integer) vorticity. The band touching EPs only appear for $\gamma^2 > t_1^2$.

Topological invariant.—The topology invariants are recently constructed in the non-Hermitian systems [92] [104] [106] [109] [120]. The Chern number defined via Berry curvature [92] [105], the vorticity defined via the complex energy [106], and the generalized Berry phase defined via the argument of effective magnetic field [104] [105] [109] are quantized. The vorticity of the topological defects in a vector field associated with the Bloch Hamiltonian is a bulk topological invariant to characterize the topological properties [115] [117], which can be generalized to non-Hermitian systems. A two-component vector field $\mathbf{F}(k) = (\langle \sigma_x \rangle, \langle \sigma_y \rangle)$ is defined through the average values of the Pauli matrices under the eigenstates of $h_0(k)$.

The topological defects in the vector field are associated with vortices (red dots) or antivortices (blue dots). The winding number $w = \oint_L (2\pi)^{-1} (\nabla \times F_x - \nabla \times F_y) \times dk$ characterizes the vorticity of the topological defects and $2\pi w$ accounts the varying direction of $\mathbf{F}(k)$ in the closed loop $L$ in the parameter plane $k = (k, t_2)$, where $F_x(y) = F_y(x)/(\sqrt{F_x^2 + F_y^2})$ and $\nabla = \partial / \partial k$. $\mathbf{F}(k)$ is depicted in Figs. 4(a) and 4(b); the winding number obtained from the vector field defined in the parameter space is in accord with that defined in the Brillouin zone of a two-dimensional (2D) brick wall lattice in the momentum space $k = (k_x, k_y)$, along one direction of the 2D lattice is system b [74]. The varying direction of the vector field $\mathbf{F}(k)$ accumulated in the loop $L$ is $\pm 2\pi (\pm \pi)$ in Fig. 4(a) [Fig. 4(b)] if L encircling a topological defect, the plus (minus) sign corresponds to the vortex (antivortex); otherwise, if L does not encircle a topological defect, the varying direction is zero.

The phase diagram is plotted in Fig. 4(c) for real $\gamma$. For $\mu \nu > 0$, the degeneracy points are at $t_1^2 - \mu \nu = 0$. As the non-Hermiticity increases, the band gap inside two high order EP’s [74] [73] with complex spectrum diminishes and closes at $t_1 = 0$ when $\gamma^2 = t_1^2$. The high order EP’s are at

FIG. 4. The vector field $\mathbf{F}(k)$ associated with $E_{b,\pm}$ of $h_0(k)$ for (a) $\mu \nu = t_1^2 - \gamma^2 > 0$ and (b) $\mu \nu = t_1^2 - \gamma^2 < 0$. The red (blue) circles indicate the topological defects with vortices (antivortices), which appear at $(k, t_2) = (0, -\sqrt{t_1^2 - \gamma^2})$ or $(\pm \pi, \sqrt{t_1^2 - \gamma^2})$ in (a) and at $(k, t_2) = (\pm \pi/2, \pm \sqrt{t_1^2 - t_2^2})$ in (b). (c) Phase diagram for real $\gamma$. Two topological zero edge states exist in the blue region $-t_2 < \mu < t_2$ for one intercell coupling $t_2$ missing. (d) Zero edge states for systems a and b under OBC. The system parameters are $N = 40$, $t_1 = 1/4$, $\gamma = 1/2$, and $t_2 = 1$. 


\( \mu \nu = 0 \) \((t_1 = \pm \gamma)\), where half of the eigenstates are two-state coalesced at energy \( t_2 \) and \(-t_2\), respectively. For \( \mu \nu < 0, t_1^2 + \mu \nu = 0 \) yields another boundary for the zero edge states determined from the band touching EPs. Two topological zero edge states exist in the regions \( \gamma^2 - t_2^2 < t_1^2 < \gamma^2 + t_2^2 \) for one intercell coupling \( t_2 \) vanishing under OBC \([148]\). As \( \gamma \) increases, the region with edge states expends when \( \gamma^2 \leq t_2^2 \), but shrinks when \( \gamma^2 > t_2^2 \).

**Topological edge states.**—The bulk topology relates to the (dis)appearance of edge states at the interfaces where topological invariant \((\nu)\) changes. We consider that the unit cells are complete \((N = 4n)\), and one intercell coupling \( t_2 \) vanishes (the Supplemental Material provides the cases of defective unit cell at system boundary \([144]\)). In system \( b \), two edge states localize on the left and right boundaries, respectively in all blue regions of Fig. 4(c). In system \( a \), the left and right edge states localize on the left and right boundaries, respectively only in region \( V \); and both two edge states localize on the right (left) boundary in regions I and III (II and IV). Figure 4(d) shows the edge states of systems \( a \) and \( b \) under OBC.

For system \( b \), the left edge state localized on the left boundary is \( \psi_{2j} = 0 \) and

\[
\psi_{2j+1} = -((\mu + \nu) + (-1)^j (\mu - \nu))/2t_2 \psi_{2j-1},
\]

at large system size limit \((N \gg 1)\). The right edge state is a left-right spatial reflection of the left edge state under symmetry protection. Anomalous edge states localize in single unit cell at system boundary at the high order EPs \((t_1^2 = \gamma^2)\) \([104, 110, 117]\). At \( t_1 = -\gamma \), the left (right) edge state is \( \psi_1 = 1 (\psi_N = 1) \); at \( t_1 = \gamma \), the left edge state is \( \psi_1 = -(+) \psi_3 = 1 \) and the right edge state is \( \psi_N = -(+) \psi_{N-2} = 1 \) when \( t_1/t_2 > 0 \) \((t_1/t_2 < 0)\).

In contrast, for system \( a \), the left edge state is \( \psi_{2j} = 0 \) and \( \psi_{2j+1} = -(\nu/t_2) \psi_{2j-1} \). The right edge state has different decay rate \(-\mu/t_2\). The edge state is \( \psi_{2j-1} = 0 \) and \( \psi_{N-2j} = -(\mu/t_2) \psi_{N+2-2j} \). The probability distributions for the two edge states are imbalanced due to the non-Hermitian asymmetric coupling. The green (red) ribbon in Fig. 4(c) indicates \( |\nu/t_2| < 1 \) \((|\mu/t_2| < 1)\), both edge states localize on the right (left) boundary. The edge states are \( \psi_1 = 1 (\psi_N = 1) \) for \( t_1/t_2 < 0 \) \((t_1/t_2 > 0)\) at the high order EPs.

**Discussion.**—The non-Hermitian asymmetric coupling can be realized through introducing a synthetic imaginary gauge field \([149, 150]\), in an array of coupled resonators consisting of primary resonators that evanescently coupled with the assistance of auxiliary resonators, the auxiliary resonators have half perimeter gain and half perimeter loss, leading to the amplification and attenuation for the coupling amplitudes in opposite tunneling directions. Alternatively, the asymmetric coupling can be realized via synthetic real gauge field and a pair of gain and loss \([151]\); the symmetric and anti-symmetric supermodes enable an asymmetric coupling between them.

Implementation of asymmetric coupling with ultracold atoms in optical lattice is possible \([121]\).

The finite size effects appear in the discrete systems. The band touching at \( t_1 = 0 \) for \( \gamma = \pm t_2 \) is subtle, two disconnected regions appear on both sides of \( k = 0 \) in the discrete systems \([117]\), the disconnection vanishes as \( N \to \infty \) \([120]\). For system \( b \) at complex \( \gamma \), the momenta \( k \) for band touching in the energy spectra are no longer \( 0, \pm \pi/2, \) or \( \pm \pi \) and may not be seen in the discrete system with small size \([144]\). The nonvanishing gap in \(|E|\) diminishes (vanishes) as system size increasing \((N \to \infty)\).

The combined chiral-inversion symmetry protects the validity of bulk-boundary correspondence, while the individual chiral and inversion symmetries are not necessarily hold separately \([144]\). The bulk-boundary correspondence is applicable when the chiral-inversion symmetry holds in the presence of non-Hermiticity \([75, 76, 84, 82]\); in contrast, it is invalid without chiral-inversion symmetry in Refs. \([116, 129]\). The system studied in Refs. \([116, 118]\) is equivalent to system \( a \) through a similar transformation \( U = e^{2i \alpha} \otimes (i \sigma_x + t_2) \). The bulk-boundary correspondence fails although all the coupling strengths are symmetric as the introduced gain and loss break the chiral-inversion symmetry; however, if the gain and loss are also alternatively introduced in the translational invariant direction, the chiral-inversion symmetry holds and the bulk-boundary correspondence recovers.

**Conclusion.**—Non-Hermiticity may alter the system topology by breaking the combined chiral-inversion symmetry of the Hermitian system, induce a topological phase transition, and lead to the breakdown of (conventional) bulk-boundary correspondence. When the chiral-inversion symmetry is fixed via alternatively introducing the non-Hermiticity, the bulk-boundary correspondence is valid. The band touching degeneracy (exceptional) points, protected by symmetry, are the topological defects with vortex or antivortex in the vector field that associated with the Bloch Hamiltonian. The vorticity of topological defects is a topological invariant, which characterizes the bulk topology and its change correctly predicts the (non)existence of topological boundary states in the non-Hermitian systems. We first reveal the roles played by symmetry and non-Hermiticity, and settle the fundamental problem of the validity of bulk-boundary correspondence in non-Hermitian systems.

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SUPPLEMENTAL MATERIAL FOR “BULK-BOUNDARY CORRESPONDENCE IN NON-HERMITIAN SYSTEMS”

Identical spectra for systems under open boundary condition

The Hamiltonian of system $\rho$ ($\rho = a, b$) under open boundary condition (OBC) is denoted as $H_{\rho,N}$, where $N$ is the system size. We have the matrices

$$H_{a,1} - EI_1 = H_{b,1} - EI_1 = (-E),$$

$$H_{a,2} - EI_2 = H_{b,2} - EI_2 = \begin{pmatrix} -E & \mu \\ \nu & -E \end{pmatrix},$$

and

$$H_{a,N} - EI_N = \begin{pmatrix} -E & \mu & \gamma & \nu \\ \nu & -E & t_2 & \gamma \\ t_2 & -E & -E & t_2 \\ \gamma & \nu & t_2 & \cdots \end{pmatrix}, H_{b,N} - EI_N = \begin{pmatrix} -E & \mu & \gamma & \nu \\ \nu & -E & t_2 & \gamma \\ t_2 & -E & -E & t_2 \\ \gamma & \nu & t_2 & \cdots \end{pmatrix},$$

where $I_N$ is the $N \times N$ identical matrix. The determinant $D_N (\rho)$ for system $\rho$ is

$$D_N (\rho) = \text{Det} \left( H_{\rho,N} - EI_N \right),$$

they satisfy a recursion relationship

$$D_{2m-1} (\rho) = (-E) D_{2m-2} (\rho) - t_2^2 D_{2m-3} (\rho),$$

$$D_{2m} (\rho) = (-E) D_{2m-1} (\rho) - \mu \nu D_{2m-2} (\rho),$$

for integer $m$ from 2 to $2n$. Equations (6)-(7) yield $D_1 (a) = D_1 (b)$ and $D_2 (a) = D_2 (b)$, we acquire $D_3 (a) = D_3 (b)$ and consequently $D_N (a) = D_N (b)$. The eigenvalues $E$ of $H_{\rho,N}$ for system $\rho$ is obtained from $D_N (\rho) = 0$; therefore, two Hamiltonians $H_a$ and $H_b$ under OBC possess identical spectra.

Topological characterization

In system $b$, the bulk topological properties relate to the (non)existence of edge states. Here we calculate the bulk topological invariant of system $b$, which is capable of characterizing the topologies of both systems $a$ and $b$ under OBC. The Bloch Hamiltonian of system $b$ is a $4 \times 4$ matrix; after a similar transformation, the Bloch Hamiltonian can be expressed in the form of $\vec{B} \cdot \vec{\sigma}$ with a two-site unit cell, then we define a vector field $\mathbf{F} (k)$ that associated with the Bloch Hamiltonian. The topological defects with vortices or antivortices in the vector field indicate the phase transition points. The vorticity of the topological defects is a topological invariant. We consider that $t_1$ and $\gamma$ are real numbers $\mu = t_1 - \gamma$ and $\nu = t_1 + \gamma$, discussions on other cases are similar following the same procedure below.

For $\mu \nu > 0$, $\mu$, $\nu$, and $\sqrt{\mu \nu}$ are positive real numbers. The Bloch Hamiltonian $H_b (k)$ under a similar transformation $U_{\mu \nu > 0} = \text{diag} \left( \sqrt{\mu}, \sqrt{\nu}, \sqrt{\mu}, \sqrt{\nu} \right)$ that only consists of diagonal elements, yields

$$U_{\mu \nu > 0} H_b (k) U_{\mu \nu > 0}^{-1} = \begin{pmatrix} 0 & \sqrt{\mu \nu} & 0 & t_2 e^{-ik} \\ \sqrt{\mu \nu} & 0 & t_2 & 0 \\ 0 & t_2 & 0 & \sqrt{\mu \nu} \\ t_2 e^{ik} & 0 & \sqrt{\mu \nu} & 0 \end{pmatrix},$$

which equals to the Bloch Hamiltonian of system $a$ with all the asymmetric couplings $\mu$ and $\nu$ replaced by the symmetric coupling $\sqrt{\mu \nu}$ and taken two unit cells as a compound unit cell. The Bloch Hamiltonian of equation (12) is rewritten in the form of

$$h_b (k) = \begin{pmatrix} 0 & \sqrt{\mu \nu} + t_2 e^{-ik} \\ \sqrt{\mu \nu} + t_2 e^{ik} & 0 \end{pmatrix}.$$
\[ h_b (k) = \vec{B} \cdot \vec{\sigma}, \] where the effective magnetic field is
\[ \vec{B} = (\sqrt{\mu \nu} + t_2 \cos k, t_2 \sin k, 0). \] (14)

Notably, in the discrete system with lattice size \( N = 4n \), the wave vector \( k \) is \( k = 2\pi m/n, m \in [1, n] \) (\( m, n \) are positive integers) for the Bloch Hamiltonian with a four-site unit cell, and the wave vector \( k \) is \( k = \pi m/n, m \in [1, 2n] \) for the Bloch Hamiltonian with a two-site unit cell.

We define a vector field \( \mathbf{F} (k) = (\langle \sigma_x \rangle, \langle \sigma_y \rangle) \) to characterize the topology of \( h_b (k) \). The eigenstates associated with \( E_{\pm} (k) = \pm \sqrt{(\mu \nu + t_2 e^{-ik}) (\mu \nu + t_2 e^{ik})} \) are
\[ \psi_{\pm} (k) = \frac{1}{\sqrt{2 \mu \nu + 2 \sqrt{\mu \nu} t_2 \cos k + t_2^2}} \left( \begin{pmatrix} \pm \sqrt{\mu \nu + t_2 e^{-ik}} \\ \sqrt{\mu \nu + t_2 e^{ik}} \end{pmatrix} \right). \] (15)

The average values of the Pauli matrices associated with the two components effective magnetic field \( \langle \sigma_{x,y} \rangle_{\pm} = \langle \psi_{\pm} (k) | \sigma_{x,y} | \psi_{\pm} (k) \rangle \) are
\[ \langle \sigma_x \rangle_{\pm} = \frac{\pm (\sqrt{\mu \nu + t_2 \cos k})}{\sqrt{\mu \nu + 2 \sqrt{\mu \nu} t_2 \cos k + t_2^2}}, \langle \sigma_y \rangle_{\pm} = \frac{\pm t_2 \sin k}{\sqrt{\mu \nu + 2 \sqrt{\mu \nu} t_2 \cos k + t_2^2}}, \] (16)

i.e., \( \langle \sigma_x \rangle_{\pm}, \langle \sigma_y \rangle_{\pm} = (B_x, B_y)/E_{\pm} \); thus, \( \langle \sigma_x \rangle_{\pm}, \langle \sigma_y \rangle_{\pm} \) reflects the topological properties of the Bloch bands and the system. The vector field \( \mathbf{F} (k) \) under either eigenstate yields the same winding number \( w = \oint (2\pi)^{-1} (\vec{F}_x \nabla \vec{F}_y - \vec{F}_y \nabla \vec{F}_x) \, dk \) in the parameter plane \( k = (k, t_2) \), where \( \vec{F}_{x\langle y \rangle} = F_{x\langle y \rangle}/\sqrt{F_x^2 + F_y^2} \) and \( \nabla = \partial/\partial k \). The phase transition occurs at \( (k, t_2) = (0, -\sqrt{\mu \nu}) \) or \( (\pm \pi, \sqrt{\mu \nu}) \), which are the band touching degeneracy points. They are topological defects in the vector field possessing integer topological charges (vortices and antivortices) as depicted in Fig. 4(a) in the Letter. The winding number \( w \) characterizing the vorticity of the topological defects, is a topological invariant.

For \( \mu \nu < 0, -\mu, \nu, \) and \( -\sqrt{\mu \nu} \) are positive real numbers. The Bloch Hamiltonian \( H_b (k) \) under a similar transformation \( U_{\mu \nu < 0} H_b (k) U_{\mu \nu < 0}^{-1} \) yields
\[ U_{\mu \nu < 0} H_b (k) U_{\mu \nu < 0}^{-1} = \begin{pmatrix} 0 & i \sqrt{-\mu \nu} & 0 & t_2 e^{-ik} \\ i \sqrt{-\mu \nu} & 0 & t_2 & 0 \\ 0 & t_2 & 0 & i \sqrt{-\mu \nu} \\ t_2 e^{ik} & 0 & i \sqrt{-\mu \nu} & 0 \end{pmatrix}, \] (17)

which is the Bloch Hamiltonian of system \( a \) with all the asymmetric couplings \( \mu \) and \( \nu \) replaced by the symmetric coupling \( i \sqrt{-\mu \nu} \) and taken two unit cells as a compound unit cell. The Bloch Hamiltonian can be rewritten as
\[ h_b (k) = \begin{pmatrix} 0 & i \sqrt{-\mu \nu} + t_2 e^{-ik} \\ i \sqrt{-\mu \nu} + t_2 e^{-ik} & 0 \end{pmatrix}. \] (18)

where the effective magnetic field is
\[ \vec{B} = (i \sqrt{-\mu \nu} + t_2 \cos k, t_2 \sin k, 0). \] (19)

the eigenvalues are \( E_{\pm} (k) = \pm \sqrt{(i \sqrt{-\mu \nu} + t_2 e^{-ik}) (i \sqrt{-\mu \nu} + t_2 e^{ik})} \); correspondingly, the eigenstates are
\[ \psi_{\pm} (k) = \frac{1}{\sqrt{\Delta}} \begin{pmatrix} \pm i \sqrt{-\mu \nu} + t_2 e^{-ik} \\ \pm i \sqrt{-\mu \nu} + t_2 e^{ik} \end{pmatrix}, \] (20)

where \( \Delta = t_2^2 - 2 \sqrt{\mu \nu} t_2 \sin k - \mu \nu + \sqrt{t_2^4 + 2 \sqrt{\mu \nu} t_2 \sin k - \mu \nu}. \)

The average values of \( \langle \sigma_{x,y} \rangle_{\pm} = \langle \psi_{\pm} (k) | \sigma_{x,y} | \psi_{\pm} (k) \rangle \) are
\[ \langle \sigma_x \rangle_{\pm} = \frac{\pm \left( e^{-2ik} t_2^2 - \mu \nu + \sqrt{e^{-2ik} t_2^4 - \mu \nu} \right)}{\Delta}, \langle \sigma_y \rangle_{\pm} = \frac{\pm i \left( e^{-2ik} t_2^2 - \mu \nu - \sqrt{e^{2ik} t_2^4 - \mu \nu} \right)}{\Delta}. \] (21)
The phase transition points are \((k, t_2) = (\pm \pi / 2, \pm \sqrt{-\mu \nu})\), which are the band touching EPs. They are topological defects in the vector field possessing half-integer topological charges (vortices and antivortices) as depicted in Fig. 4(b) in the Letter.

The two-dimensional (2D) brick wall lattice is schematically illustrated in Supplementary Figure 5. In the momentum space, the Bloch Hamiltonians \(H_a^{(2D)}(k)\) and \(H_b^{(2D)}(k)\) are

\[
H_a^{(2D)}(k) = \begin{pmatrix}
0 & 2 \mu \cos (k_y) & 0 & t_2 e^{-ik_x} \\
2 \nu \cos (k_y) & 0 & t_2 e^{ik_x} & 0 \\
t_2 e^{ik_x} & t_2 e^{-ik_x} & 0 & 2 \nu \cos (k_y) \\
0 & 0 & 2 \mu \cos (k_y) & 0
\end{pmatrix},
\]

\[\tag{22}\]

\[
H_b^{(2D)}(k) = \begin{pmatrix}
0 & 2 \mu \cos (k_y) & 0 & t_2 e^{-ik_x} \\
2 \nu \cos (k_y) & 0 & t_2 e^{ik_x} & 0 \\
t_2 e^{ik_x} & t_2 e^{-ik_x} & 0 & 2 \nu \cos (k_y) \\
0 & 0 & 2 \mu \cos (k_y) & 0
\end{pmatrix}.
\]

\[\tag{23}\]

The vortices and antivortices associated with the phase transition points in the Brillouin zone in the \(k_x - k_y\) space are shown in Supplementary Figures 5(c) and 5(d), which are in accords with that revealed in Figs. 4(a) and 4(b) in the Letter.

Under a similar transformation \(U_b^{(2D)} = \text{diag} (\sqrt{\mu}, \sqrt{\nu}, \sqrt{\mu}, \sqrt{\nu})\), the Bloch Hamiltonian \(H_b^{(2D)}(k)\) changes into

\[
U_b^{(2D)} H_b^{(2D)}(k) U_b^{(2D)-1} = \begin{pmatrix}
0 & 2 \sqrt{\mu \nu} \cos k_y & 0 & t_2 e^{ik_x} \\
2 \sqrt{\mu \nu} \cos k_y & 0 & t_2 e^{-ik_x} & 0 \\
t_2 e^{ik_x} & t_2 e^{-ik_x} & 0 & 2 \sqrt{\mu \nu} \cos k_y \\
0 & 0 & 2 \sqrt{\mu \nu} \cos k_y & 0
\end{pmatrix},
\]

\[\tag{24}\]

and the corresponding two-site unit cell Bloch Hamiltonian is

\[
h_b^{(2D)} = \begin{pmatrix}
0 & 2 \sqrt{\mu \nu} \cos k_y + t_2 e^{ik_x} \\
2 \sqrt{\mu \nu} \cos k_y + t_2 e^{-ik_x} & 0
\end{pmatrix}.
\]

\[\tag{25}\]

The eigenvalues are \(E_{b, \pm}^{(2D)} = \pm \sqrt{t_2^2 + 4 \sqrt{\mu \nu} \cos k_x \cos k_y + 4 \nu \mu \cos^2 k_y}\).

**Edge states for systems with defective unit cell at boundary**

For system \(b\) with an even site number (total site number \(N = 4n - 2\)), we consider that \(H_b\) under OBC with two sites [inside the red rectangle in Fig. 1(b) in the Letter] at the right boundary are missing. Two zero edge states localize at the left and the right boundaries, respectively. The left edge state is Eq. (5) in the Letter. The right edge state localized at the right boundary is \(\psi_{2j-1} = 0\) and

\[
\psi_{N-2j} = -[(\nu + \mu) + (-1)^j (\nu - \mu)](2t_2) \psi_{N+2-2j}.
\]

\[\tag{26}\]
at large system size limit \((N \gg 1)\). For the anomalous edge states at the high order EPs \((t_1^2 = \gamma^2)\), they are localized at single unit cell at system boundary. For \(t_1 = -\gamma\), the left (right) edge state is \(\psi_1 = 1 (\psi_N = 1)\); and for \(t_1 = \gamma\), the right edge state is \(\psi_N = 1\); the left edge state is \(\psi_1 = - (+) \psi_3 = 1\) for \(t_1/t_2 > 0 (t_1/t_2 < 0)\).

For system \(b\) with an odd site number, the energy spectra are depicted in Supplementary Figures \(6(a)\)–\(6(c)\), the edge state is depicted in Supplementary Figures \(6(d)\)–\(6(f)\). Only one zero edge state exists in this situation. Considering that the unit cell at the right boundary is defective. In the situation that \(|\mu\nu| < t_2^2\), the edge state localizes at the left boundary, the wave function is Eq. (5) in the Letter; in the situation that \(|\mu\nu| > t_2^2\), for the system with site number \(N = 4n - 1\), the edge state localized at the right boundary is \(\psi_{2j} = 0\) and

\[
\psi_{N-2j} = -(2t_2)/[\left(\mu + \nu\right) + (-1)^j \left(\mu - \nu\right)]\psi_{N+2-2j} \tag{27}
\]

for the system with site number \(N = 4n - 3\), the edge state localized at the right boundary is \(\psi_{2j} = 0\) and

\[
\psi_{N-2j} = -(2t_2)/[\left(\nu + \mu\right) + (-1)^j \left(\nu - \mu\right)]\psi_{N+2-2j} \tag{28}
\]

For the anomalous edge states at the high order EPs \((t_1^2 = \gamma^2)\) and the systems with site numbers \(N = 4n - 1\) and \(4n - 3\), the left edge state is \(\psi_1 = - (+) \psi_3 = 1\) for \(t_1/t_2 > 0 (t_1/t_2 < 0)\) at \(t_1 = \gamma\) and \(\psi_1 = 1\) at \(t_1 = -\gamma\).

![FIG. 6. (a-c) Energy spectra of system \(b\) with \(N = 39\) at parameters \(\gamma = 1/2\) and \(t_2 = 1\). The zero edge state at (d) \(t_1 = 1/4\), (e) \(t_1 = 1/2\), and (f) \(t_1 = 3/2\).](image)

In contrast, for system \(a\) with an odd site number has a defective unit cell at the right boundary, only one zero state exists. The right boundary state is \(\psi_{2j} = 0\) and \(\psi_{N-2j} = (-t_2/\nu) \psi_{N+2-2j}\) when \(|t_2| < \sqrt{\mu\nu}\). At the high order EPs, the zero state localizes at one site on the left boundary \(\psi_1 = 1\) for \(t_1 = -\gamma\); and the zero state is extended, being \(\psi_{2j} = 0\) and \(\psi_{2j-1} = - (+) \psi_{2j+1}\) for \(t_1 = \gamma\) at \(t_1/t_2 > 0 (t_1/t_2 < 0)\).

**Energy spectra for complex asymmetric coupling**

For system \(b\) at \(\gamma = \sqrt{1/2} e^{i\pi/4}\), the phase transition points are \(t_1 = \pm \sqrt{3/4} \approx 0.93\) and \(|\cos (k)| = \sqrt{(2 + \sqrt{3})/2}\). The band touching degeneracy points may not be seen in the discrete system with small system size due to the finite number of discrete \(k\). The energy spectra for \(\gamma = \sqrt{1/2} e^{i\pi/4}\) are depicted in Supplementary Figure \(7\) for \(N = 40\). The nonvanishing gap in \(|E|\) shown inside the green circles in Supplementary Figure \(7(a)\) is a finite size effect of the discrete system; as \(N\) increases, the gap vanishes and the band touching degeneracy points reveal.

![FIG. 7. Energy spectra of system \(b\) under (a) PBC and (b) OBC. The parameters are \(N = 40, \gamma = \sqrt{1/2} e^{i\pi/4}\), and \(t_2 = 1\).](image)
Chiral-inversion symmetric systems

System $b'$ is system $b$ with the asymmetric couplings $(\nu, \mu)$ in the red unit cell [Fig. 1(b) in the Letter] with an additional minus sign in front $(\nu, \mu)$ substituted by $(-\nu, -\mu)$, the Bloch Hamiltonian of system $b'$ reads

$$H_{b'}(k) = \begin{pmatrix}
0 & \mu & 0 & t_2 e^{ik} \\
\nu & 0 & t_2 & 0 \\
0 & t_2 & 0 & -\nu \\
t_2 e^{-ik} & 0 & -\mu & 0
\end{pmatrix}.$$  \hspace{2cm} (29)

For even $n$, systems $b$ and $b'$ in the real-space are connected through a similar transformation

$$U_{b'b} = P_n/2 \otimes \sigma_y \otimes \left[(\sigma_x + i\sigma_y) \otimes (i\sigma_y - \sigma_x) \otimes \sigma_x\right]/2,$$  \hspace{2cm} (30)

that $U_{b'b}H_{b'}U_{b'}^\dagger = H_b$. Therefore, systems $b$ and $b'$ have identical band structures and topological properties. System $b'$ has the combined chiral-inversion symmetry that $(\mathcal{S}\mathcal{P}) H_{b'}(k) (\mathcal{S}\mathcal{P})^{-1} = -H_{b'}(-k)$, where $\mathcal{S}\mathcal{P} = \sigma_y \otimes \sigma_x$; and $U_{\mathcal{S}\mathcal{P}} H_{b'} U_{\mathcal{S}\mathcal{P}}^\dagger = -H_{b'}$, where $U_{\mathcal{S}\mathcal{P}} = P_n \otimes (\sigma_y \otimes \sigma_x)$. The chiral symmetry is satisfied that $\mathcal{S}H_{b'} \mathcal{S}^{-1} = -H_{b'}$, where $\mathcal{S} = I_{2n} \otimes \sigma_z$, but the inversion symmetry is violated. System $b$ with alternative on-site gain and loss $\{i\Gamma, -i\Gamma, i\Gamma, -i\Gamma\}$ introduced in the four-site unit cell possesses the chiral-inversion symmetry that $(\mathcal{S}\mathcal{P}) H_b(k) (\mathcal{S}\mathcal{P})^{-1} = -H_b(-k)$, where $\mathcal{S}\mathcal{P} = \sigma_x \otimes \sigma_y$; and $U_{\mathcal{S}\mathcal{P}} H_b U_{\mathcal{S}\mathcal{P}}^\dagger = -H_b$, where $U_{\mathcal{S}\mathcal{P}} = P_{2n} \otimes \sigma_y$. Notably, both the chiral symmetry and the inversion symmetry are violated. The energy spectra under PBC and OBC are depicted in Supplementary Figures 8(a) and 8(b), respectively.

Their energy spectra under OBC and PBC are in Supplementary Figures 8(b) and 8(c) for system $a$ with $\{i\Gamma, -i\Gamma\}$ introduced in the unit cell, which has identical (different) spectrum under OBC (PBC) with that of system $b$ composed by introducing $\{i\Gamma, -i\Gamma, i\Gamma, -i\Gamma\}$ aiming to fix the chiral-inversion symmetry in system $a$. Notably, the band touching degeneracy (exceptional) points in the energy spectra of the systems under PBC and OBC are in accords with each other; the system boundary does not alter most of the bulk states, the bulk states are all extended states, and the non-Hermitian skin effect is absent.

FIG. 8. Energy spectrum for system $b$ with staggered gain and loss $\{i\Gamma, -i\Gamma, i\Gamma, -i\Gamma\}$ under (a) PBC and (b) OBC. (c) Energy spectrum for system $a$ with staggered gain and loss $\{i\Gamma, -i\Gamma\}$ under PBC, the corresponding OBC spectrum is in (b). The parameters are $N = 40$, $\gamma = 1/2$, $\Gamma = 1/2$, and $t_2 = 1$. 