Bloch Band Theory for Non-Hermitian Systems

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In spatially periodic Hermitian systems, such as electronic systems in crystals, the band structure is described by the band theory in terms of the Bloch wave functions, which reproduces energy levels for large systems with open boundaries. In this paper, we establish a generalized Bloch band theory in one-dimensional spatially periodic tight-binding models. We show how to define the Brillouin zone in non-Hermitian systems. From this Brillouin zone, one can calculate continuum bands, which reproduce the band structure in an open chain. As an example we apply our theory to the non-Hermitian SSH model. We also show the bulk-edge correspondence between the winding number and existence of the topological edge states.

The band theory in crystals is fundamental for describing electronic structures. By introducing the Bloch wave vector $\mathbf{k}$, the band structure calculated within a unit cell reproduces that of a large crystal with open boundaries. Here it is implicitly assumed that the electronic states are almost equivalent between a system with open boundaries and that with the periodic boundaries, represented by the Bloch wave function with real $\mathbf{k}$. It is because the electronic states extend over the system.

Recently, non-Hermitian systems, which are described by non-Hermitian Hamiltonians, have been attracting much attention. These systems have been both theoretically and experimentally studied in many fields of physics. In particular, the bulk-edge correspondence has been intensively studied in topological systems. In contrast to Hermitian systems, it seems to be violated in some cases. The reasons for this violation have been under debate.

One of the controversial points is that in many previous works, the Bloch wave vector has been treated as real in non-Hermitian systems similarly to Hermitian ones. In Ref. 83, it was proposed that in one-dimensional (1D) non-Hermitian systems, the wave number $k$ becomes complex. The value of $\beta \equiv e^{ik}$ is confined on a loop on the complex plane, and this loop is a generalization of the Brillouin zone in Hermitian systems. In non-Hermitian systems, the wave functions in large systems with open boundaries do not necessarily extend over the bulk, but are localized at the either end of the chain unlike those in Hermitian systems. Thus far, how to obtain the generalized Brillouin zone has been known only for simple systems.

In this paper, we establish a generalized Bloch band theory to calculate continuum bands in a 1D tight-binding model. First of all, we establish a way to determine the generalized Brillouin zone $C_\beta$ for $\beta \equiv e^{ik}$, $k \in \mathbb{C}$. This determines continuum bands, which reproduce band structure for a large crystal with open boundaries. We introduce the “Bloch” Hamiltonian $H(\mathbf{k})$ and rewrite it in terms of $\beta$ as $H(\beta)$. Then the characteristic equation $f(\beta, E) = 0$, which is an eigenvalue equation for $H(\beta)$, is an algebraic equation for $\beta$, and let $2M$ be the degree of the equation. We find that when the characteristic equation has solutions $\beta_i (i = 1, \cdots, 2M)$ with $|\beta_1| \leq |\beta_2| \leq \cdots \leq |\beta_{2M-1}| \leq |\beta_{2M}|$, $C_\beta$ is given by the trajectory of $\beta_M$ and $\beta_{M+1}$ under a condition $|\beta_M| = |\beta_{M+1}|$. Furthermore, one can get continuum bands by diagonalizing $H(\beta)$ with $\beta \in C_\beta$. We note that in Hermitian systems, this condition reduces to $C_2 : |\beta| = 1$, meaning that the Bloch wave number $k$ being real. In Ref. 83 the case with $M = 1$ has been solved, and we give a nontrivial extension into general $M$.

A byproduct of our theory is that one can prove the bulk-edge correspondence. The bulk-edge correspondence has been discussed, but in most cases it has not been shown rigorously but by observation on some particular cases, together with an analogy to Hermitian systems. In fact it shows that the bulk-edge correspondence for the real Bloch wave vector cannot be true in non-Hermitian systems. In this paper, we show the bulk-edge correspondence in the non-Hermitian SSH model with the generalized Brillouin zone, and discuss the relationship between a topological invariant in the bulk and existence of the edge states.

We start with a 1D tight-binding model, with its Hamiltonian given by

$$H = \sum_{n} \sum_{i=-N}^{N} \sum_{\mu} t_{i,\mu} c_{n+1,\mu}^{\dagger} c_{n,\mu},$$

where $N$ represents the range of the hopping and $q$ represents internal degrees of freedom per unit cell. This Hamiltonian can be non-Hermitian, meaning that $t_{i,\mu}^{*}$ is not necessarily equal to $t_{i,\mu}^{*}$. Then one can write the real-space eigen-equation as $H|\psi\rangle = E|\psi\rangle$, where the eigenvector is written as $|\psi\rangle = (\psi_{1,1}, \cdots, \psi_{1,q}, \cdots, \psi_{L,1}, \cdots, \psi_{L,q})^T$ in an open chain. Thanks to the spatial periodicity, one can write the eigenvector as a linear combination:

$$\psi_{n,\mu} = \sum_{j} \phi_{n,\mu}^{(j)}, \quad \phi_{n,\mu}^{(j)} = (\beta_j)^{n} \phi_{\mu}^{(j)}, \quad (\mu = 1, \cdots, q).$$

By imposing that $\phi_{n,\mu}^{(j)}$ is a bulk eigenstate, one can obtain
the characteristic equation for $\beta = \beta_j$ as

$$f(\beta, E) = 0.$$  \hfill (3)

This characteristic equation is nothing but an eigenvalue equation for the generalized Bloch Hamiltonian $H(\beta)$, and therefore it can be obtained similarly to Hermitian cases. Equation (3) is an algebraic equation for $\beta$ with an even degree $2M$ in general cases.

One can see from Eq. (2) that $\beta$ corresponds to the Bloch wave number $k \in \mathbb{R}$ via $\beta = e^{ik}$ in Hermitian systems. The bulk-band structure for reality of $k$ reproduces the band structure of a long open chain. When extending this idea to non-Hermitian systems, we should choose the values of $\beta$ such that the bands of the Hamiltonian $H(\beta)$ reproduce those of a long open chain (Fig. 1). The levels are discrete in a finite open chain, and as the system size becomes larger, the levels become dense and asymptotically form continuum bands (Fig. 1). Therefore in order to find the generalized Brillouin zone $C_{\beta}$, one should consider asymptotic behavior of level distributions in an open chain in the limit of a large system size. In Hermitian systems $|\beta|$ is equal to unity, meaning that the eigenstates extend over the bulk. On the other hand, in non-Hermitian systems, $|\beta|$ is not necessarily unity, and these states may be localized at an either end of the chain. Therefore these bands cannot be called bulk bands, but should be called continuum bands. These states are incompatible with the periodic boundary conditions. The continuum bands are formed by changing $\beta$ continuously along $C_{\beta}$ as we show later.

We find how to determine the generalized Brillouin zone $C_{\beta}$, which determines the continuum bands. Here we number the solutions $\beta_i$ $(i = 1, \cdots, 2M)$ of Eq. (2) so as to satisfy $|\beta_1| \leq |\beta_2| \leq \cdots \leq |\beta_{2M-1}| \leq |\beta_{2M}|$. We find that the condition to get the continuum bands can be written as

$$|\beta_M| = |\beta_{M+1}|,$$  \hfill (4)

and the trajectory of $\beta_M$ and $\beta_{M+1}$ gives $C_{\beta}$. When $M = 1$, the two solutions of the quadratic equation share same absolute values, as has been proposed in Ref. 83; nonetheless, for general $M$, its condition has not been known so far. In Hermitian systems, we can prove that Eq. (4) becomes $|\beta_M| = |\beta_{M+1}| = \frac{2}{2M}$, and $C_{\beta}$ is a unit circle $|\beta| = 1$.

To get Eq. (4), we focus on boundary conditions in an open chain. Here we outline the discussion to show Eq. (4), and the detailed discussion is given by Ref. 82. We impose the wave function Eq. (2) to represent an eigenstate. Apart from the positions near the two ends, it leads to the characteristic equation Eq. (3). The boundary conditions give another constraint onto the values of $\beta_i$ $(i = 1, \cdots, 2M)$, in a form of an algebraic equation. We now suppose the system size $L$ to be quite large, and consider a condition to achieve a densely distributed levels (Fig. 1). The equation consists of terms of the form $(\beta_1 \beta_2 \cdots \beta_M)^{L+1}$. When $|\beta_M| \neq |\beta_{M+1}|$, there is only one leading term proportional to $(\beta_{M+1} \cdots \beta_{2M})^{L+1}$, which does not allow continuum bands. Only when $|\beta_M| = |\beta_{M+1}|$, there are two leading terms proportional to $(\beta_M \beta_{M+2} \cdots \beta_{2M})^{L+1}$ and to $(\beta_{M+1} \beta_{M+2} \cdots \beta_{2M})^{L+1}$. In such a case, the relative phase between $\beta_M$ and $\beta_{M+1}$ can be changed almost continuously for a large $L$, producing the continuum bands. We note that our condition Eq. (4) is independent of any boundary conditions of an open chain. In Ref. 83, it was proposed that the continuum bands require $|\beta_i| = |\beta_j|$. Nonetheless, it is not sufficient; except for the case $|\beta_M| = |\beta_{M+1}|$, it does not allow the continuum bands.

We apply Eq. (4) to the non-Hermitian SSH model as

FIG. 1. Schematic figure of the band structure (a) in a finite open chain with various system sizes $L$, and (b) of the generalized Bloch Hamiltonian. The vertical axis represents the distribution of the complex energy $E$.

FIG. 2. (a) Non-Hermitian SSH model. The dotted boxes indicate the unit cell. (b)-(d) Generalized Brillouin zone $C_{\beta}$ of this model. The values of the parameters are (b) $t_2 = 1, t_3 = 1/5, \gamma_1 = 4/3$, and $\gamma_2 = 0$; (b-1): $t_1 = 1.1$ and (b-2): $t_1 = -1.1, (c) t_1 = 0.3, t_2 = 1.1, t_3 = 1/5$, and $\gamma_1 = 0$; (c-1): $\gamma_2 = 4/3$ and (c-2): $\gamma_2 = -4/3$, and (d) $t_2 = 0.5, t_3 = 1/5, \gamma_1 = 5/3$, and $\gamma_2 = 1/3$; (d-1): $t_1 = 0.3$ and (d-2): $t_1 = -0.3$. 

shown in Fig. 2 (a). It is given by
\[
H = \sum_n \left[ \left( t_1 + \frac{\gamma_1}{2} \right) c_{n,A}^\dagger c_{n,B} + \left( t_1 - \frac{\gamma_1}{2} \right) c_{n,B}^\dagger c_{n,A} + \left( t_2 + \frac{\gamma_2}{2} \right) c_{n,B}^\dagger c_{n+1,A} + \left( t_2 - \frac{\gamma_2}{2} \right) c_{n+1,A}^\dagger c_{n,B} + t_3 \left( c_{n,A}^\dagger c_{n+1,B} + c_{n+1,B}^\dagger c_{n,A} \right) \right], \tag{5}
\]
where \( t_1, t_2, t_3, \gamma_1, \) and \( \gamma_2 \) are real. The generalized Bloch Hamiltonian \( H(\beta) \) can be obtained by a replacement \( e^{ik} \to \beta \), similarly to Hermitian systems, as
\[
H(\beta) = R_+(\beta) \sigma_+ + R_-(\beta) \sigma_-,
\tag{6}
\]
where \( \sigma_{\pm} = (\sigma_x \pm i \sigma_y) / 2 \), and \( R_{\pm}(\beta) \) are given by
\[
R_+(\beta) = \left( t_2 - \frac{\gamma_2}{2} \right) \beta^{-1} + \left( t_1 + \frac{\gamma_1}{2} \right) + t_3 \beta, \quad R_-(\beta) = t_3 \beta^{-1} + \left( t_1 - \frac{\gamma_1}{2} \right) + \left( t_2 + \frac{\gamma_2}{2} \right) \beta. \tag{7}
\]
Therefore the characteristic equation can be written as \( R_+(\beta) R_-(\beta) = E^2 \), which is a quartic equation for \( \beta \), i.e. \( M = 2 \), having four solutions \( \beta_i \) \( (i = 1, \cdots, 4) \). Then Eq. (6) is given by \( |\beta_2| = |\beta_3| \). \( w_+ \) takes both the values more than and less than 1. Secondly, \( C_\beta \) can be a unit circle even for non-Hermitian cases, for example when \( t_1 = t_3 = \gamma_2 = 0 \). Finally, \( C_\beta \) can have cusps, corresponding to the cases with three solutions share the same absolute value.\(^\text{58,59}\)

We calculate the winding number \( w \) for the Hamiltonian Eq. (6). Thanks to the chiral symmetry, \( w \) can be defined as
\[
w = -\frac{w_+ - w_-}{2}, \quad w_{\pm} = \frac{1}{2\pi} \arg R_{\pm}(\beta)|_{C_\beta}, \tag{8}\]
where \( \arg R_{\pm}(\beta)|_{C_\beta} \) means the change of the phase of \( R_{\pm}(\beta) \) as \( \beta \) goes along the generalized Brillouin zone \( C_\beta \) in the counterclockwise way. It was proposed that \( w \) corresponds to the presence or absence of the topological edge states.\(^\text{60}\)

We show how the gap closes in our model. It closes when \( E = 0 \), i.e. \( R_+(\beta) = 0 \) or \( R_-(\beta) = 0 \). Let \( \beta = \beta_0^i \) \( (i = 1, 2, a = \pm, -) \) denote the solutions of the equation \( R_\pm(\beta) = 0 \) with \( |\beta_i^+| \leq |\beta_i^-| \). When \( E = 0 \) is in the continuum bands, Eq. (4) should be satisfied for the four solutions \( \beta_0^i \) \( (i = 1, 2) \). It can be classified into two cases, (a) \( |\beta_1^+| \leq |\beta_1^-| = |\beta_{1}^{\ast a}| \leq |\beta_2^-| \) \( (a = \pm, -) \), and (b) \( |\beta_1^+| \leq |\beta_{1}^{\ast a}| = |\beta_2^-| \leq |\beta_2^-| \) \( (a = +, -) \). In the case (a), as one changes one parameter, the gap closes at \( E = 0 \) and \( w_+ \) and \( -w_- \) change by one at the same time, giving rise to the change of the winding number by unity. On the other hand, in the case (b), only one of the two coefficients \( R_{\pm}(\beta) \) becomes zero, and it represents an exceptional point.

We obtain the phase diagram on the \( t_1-t_2 \) plane in Fig. 3 (a) and one on the \( \gamma_1-\gamma_2 \) plane in Fig. 3 (a). In these phase diagrams, the winding number \( w \) is 1 in the blue region. By definition, \( w \) changes only when \( R_{\pm}(\beta) = 0 \) on the generalized Brillouin zone \( C_\beta \), and the gap closes. The energy bands in a finite open chain calculated along the black arrow in Fig. 3 (a) are shown in Fig. 3 (d), and one can confirm that the edge states appear in the region where \( w = 1 \). In addition, the continuum bands using \( C_\beta \) (Fig. 3 (c)) agree with these energy bands. In Fig. 4 (b), we give the energy bands calculated along the green arrow in Fig. 4 (a), and the edge states appear similarly to Fig. 3 (d). On the other hand, the system has the exceptional points in the orange region. The phase with the exceptional points extends over a finite region.\(^\text{61}\)

We discuss the bulk-edge correspondence in our model. The loops \( \ell_\pm \) drawn by \( R_{\pm}(\beta) \) on the \( R \) plane are shown in Fig. 3 (c) and Figs. 4 (c) and (d) for certain values of the parameters. Both in Fig. 3 (c) and in Fig. 4 (c), the system has the winding number \( w = 1 \) since both \( \ell_+ \) and \( \ell_- \) surround the origin \( O \), leading to \( w_+ = -1 \) and \( w_- = 1 \). In Fig. 4 (a), one can continuously change the values of the parameters to the Hermitian limit, \( \gamma_1, \gamma_2 \to 0 \), while keeping the gap open and \( w \) remain 1. The same is true for Fig. 3 (a). Therefore by following the proof in Hermitian cases,\(^\text{62}\) one can prove the bulk-edge correspondence even for the non-Hermitian cases, and
FIG. 4. Phase diagram and bulk-edge correspondence with wave number $k$ for obtaining the continuum bands. Here the Bloch systems. Our conclusion, $|\beta| = 1$, is physically reasonable in several aspects. First, it is independent of any boundary conditions. Thus for a long open chain, irrespective of any boundary conditions, the spectrum asymptotically approaches the same continuum bands calculated from $C_\beta$. Second, it reproduces the known result in the Hermitian limit, i.e. $|\beta| = 1$. Third, the form of the condition is invariant under a replacement $\beta \rightarrow 1/\beta$. Suppose the numbering of the sites is reversed by putting $n' = L+1-n$ for the site index $n(=1, \cdots, L)$; then $\beta$ becomes $\beta' = 1/\beta$, but the form of the condition is invariant: $|\beta_{M}^{R}| = |\beta_{M+1}^{L}|$.

Through this definition of the continuum bands, one can show the bulk-edge correspondence without ambiguity by defining the winding number $w$ from the generalized Brillouin zone in 1D systems with chiral symmetry. Indeed we showed that the zero-energy states appear in the non-Hermitian SSH model when $w$ takes non-zero values, and also revealed that these states correspond to topological edge states. It is left for future works how to calculate the continuum bands for systems with other symmetries.

The construction of the generalized Brillouin zone can be extended to higher dimensions as well. In two-dimensional systems, we introduce the two parameters $\beta^x(=e^{ik_x})$ and $\beta^y(=e^{ik_y})$. Then the characteristic equation $f(\beta^x, \beta^y, E) = 0$ is an algebraic equation for $\beta^x$ and $\beta^y$. If we fix $\beta^y$, this system can be regarded as a 1D system, and the criterion is given by $|\beta_{M_{\epsilon}}^{x}| = |\beta_{M_{\epsilon}+1}^{x}|$, where $2M_{\epsilon}$ is the degree of the characteristic equation for $\beta^x$. The same is true for $\beta^y$. Thus we can get the conditions for the continuum bands. Nevertheless, it is still an open question how to determine the generalized Brillouin zone in higher dimensions.

Some previous works which assume reality of $k$ require further investigations. For example, the tight-binding model in Ref. 74 is equivalent to our model with $t_3 = 0$. Within our theory, it has neither exceptional points nor anomalous edge states, as opposed to Ref. 74.

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Supplemental Material

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I. DERIVATION OF THE CONDITION FOR CONTINUUM BANDS

We find how to determine the generalized Brillouin zone \(C_B\), which determines the continuum bands. Here we number the \(2M\) solutions in the characteristic equation \(f(\beta, E) = 0\) so as to satisfy

\[
|\beta_1| \leq |\beta_2| \leq \cdots \leq |\beta_{2M-1}| \leq |\beta_{2M}|. \quad (S1)
\]

We find that the condition to get the continuum bands can be written as

\[
|\beta_M| = |\beta_{M+1}|. \quad (S2)
\]

We note that Eq. \(S2\) was proposed in Ref. \(^1\) in the case of \(M = 1\), but for general \(M\) its condition has not been known so far. To get Eq. \(S2\), we focus on boundary conditions in a finite open chain. The wave functions satisfying the boundary conditions are given by

\[
\psi_{n,\mu} = \sum_{j=1}^{2M} (\beta_j)^n \phi_{\mu}^{(j)}, \quad (\mu = 1, \cdots, q). \quad (S3)
\]

The equations from the boundary conditions include the \(2qM\) unknown variables \(\phi_{\mu}^{(j)}\). The real-space eigen-equation \(H \left| \psi \right\rangle = E \left| \psi \right\rangle\) fixes the ratio between the values of \(\phi_{\mu}^{(j)}\) sharing the same value of \(j\). Therefore one can reduce the \(2qM\) variables to the \(2M\) variables \(\phi_{\mu}^{(j)}\) with a single value of \(\mu\), e.g. \(\mu = 1\). As a result, we can get a set of equations for the \(2M\) variables \(\phi_{1}^{(j)} (j = 1, \cdots, 2M)\):

\[
A \begin{pmatrix}
\phi_{1}^{(1)} \\
\vdots \\
\phi_{1}^{(2M)}
\end{pmatrix} = 0, \quad (S4)
\]

where \(A\) is a \(2M \times 2M\) matrix. Existence of its nontrivial solutions requires

\[
\det A = 0. \quad (S5)
\]

The form of the matrix \(A\) depends on the boundary conditions and the system size. An example of these equations are given in Eqs. \(S20\) - \(S22\).

Equation \(S3\) is an algebraic equation for \(\beta_j (j = 1, \cdots, 2M)\). By solving Eqs. \(S4\) and \(S5\) one can calculate eigenenergies of the system with open boundaries. One cannot analytically solve these equations for a general system size. Nonetheless, our aim is to see how the solutions for a large system size form the continuum bands. Therefore we suppose the systems size to be quite large, and consider a condition to achieve densely distributed levels. We find that Eq. \(S5\) is expressed in a form

\[
\sum_{S} g(\beta_{S1}, \cdots, \beta_{S2M}) (\beta_{S(M+1)} \cdots \beta_{S(2M)})^{L+1} = 0 \quad (S6)
\]

where \(L\) is the number of unit cells in an open chain, the sum is taken over all the permutations \(S\) for \(2M\) objects, and \(g\) is a function of the \(2M\) variables dependent on the boundary conditions but independent of \(L\). We now consider behavior of its solution for large \(L\). When \(|\beta_M| \neq |\beta_{M+1}|\), there is only one leading term proportional to \((\beta_{M+1} \cdots \beta_{2M})^{L+1}\) in Eq. \(S6\) in the limit of a large \(L\). Thus it leads to a single equation for \(\beta_j (j = 1, \cdots, 2M)\), which does not allow continuum bands. When \(|\beta_M| = |\beta_{M+1}|\), there are two leading terms proportional to \((\beta_{M+1} \beta_{M+2} \cdots \beta_{2M})^{L+1}\) and to \((\beta_{M+1} \beta_{M+2} \cdots \beta_{2M})^{L+2}\). In such a case, we can expect that the relative phase between \(\beta_M\) and \(\beta_{M+1}\) can be changed almost continuously for a large \(L\), producing the continuum bands. We can see this for a specific example in Sec. \(III\) in this Supplemental Material. We note that our condition Eq. \(S2\) is independent of any boundary conditions.

II. GENERALIZED BRILLOUIN ZONE IN HERMITIAN SYSTEMS

We prove that the generalized Brillouin zone becomes a unit circle in Hermitian systems. In the following, we assume that the characteristic equation \(f(\beta, E) = 0\) is an algebraic equation for \(\beta\) of \(2M\)-th degree. In Hermitian systems, it can be written as

\[
\sum_{i=-M}^{M} a_i \beta^i = 0, \quad (S7)
\]

where \(a_{-i} = a_i^* (i = 1, \cdots, M)\) and \(a_0\) is real. These coefficients are functions of the eigenenergy \(E\) and the hopping terms included in the tight-binding models. Here the eigenenergy \(E\) is real due to Hermiticity of the Hamiltonian. Equation \(S7\) has \(2M\) solutions, and they are numbered so as to satisfy

\[
|\beta_1| \leq |\beta_2| \leq \cdots \leq |\beta_{2M-1}| \leq |\beta_{2M}|. \quad (S8)
\]
Since one can rewrite Eq. (S7) as
\[
\sum_{i=-M}^{M} (a_i)^* (\beta^*)^{-i} = \sum_{i=-M}^{M} a_i (\beta^*)^{-i} = 0,
\]  
(S9)
the solutions always appear in pairs: \((\beta, 1/\beta^*)\), and we get \(\beta_{2M+1-j} = 1/\beta^*_j\). In particular, one can get the relationship between \(\beta_M\) and \(\beta_{M+1}\) as \(\beta_{M+1} = 1/\beta^*_M\). Therefore the condition for the continuum bands \(|\beta_M| = |\beta_{M+1}| = 1\) can be rewritten as
\[
|\beta_M| = |\beta_{M+1}| = 1.
\]  
(S10)
Thus we can conclude that the generalized Brillouin zone becomes a unit circle in Hermitian systems.

III. NON-HERMITIAN SSH MODEL

A. Characteristic equation

We give the non-Hermitian SSH model as shown in Fig. S1. The Hamiltonian can be written as
\[
H = \sum_n \left[ (t_1 + \frac{\gamma_1}{2}) c_i^{\dagger} n_A c_{n,B} + (t_1 - \frac{\gamma_1}{2}) c_i^{\dagger} c_{n,A} + (t_2 + \frac{\gamma_2}{2}) c_i^{\dagger} n_B c_{n+1,A} + (t_2 - \frac{\gamma_2}{2}) c_i^{\dagger} c_{n+1,B} + t_3 (c_i^{\dagger} n_A c_{n+1,B} + c_i^{\dagger} n_B c_{n,A}) \right],
\]  
(S11)
where \(t_1, t_2, t_3, \gamma_1\), and \(\gamma_2\) are real for simplicity. Eigenvectors are written as \(|\psi\rangle = (\psi_{1,A}, \psi_{1,B}, \psi_{2,L,A}, \psi_{2,L,B})^T\) in an open chain. Then we can explicitly write the equation for \(\psi_{n,\mu}\) as
\[
\begin{aligned}
(t_2 - \frac{\gamma_2}{2}) \psi_{n-1,B} + (t_1 + \frac{\gamma_1}{2}) \psi_{n,B} + t_3 \psi_{n+1,B} &= E \psi_{n,A}, \\
t_3 \psi_{n-1,A} + (t_1 - \frac{\gamma_1}{2}) \psi_{n,A} + (t_2 + \frac{\gamma_2}{2}) \psi_{n+1,A} &= E \psi_{n,B},
\end{aligned}
\]  
(S12)
Here we take the ansatz for the wave function as a linear combination:
\[
\psi_{n,\mu} = \sum_j \phi_{n,\mu}^{(j)} \phi_{x,\mu}^{(j)} = (\beta_j)^n \phi_{x,\mu}^{(j)}, \quad (\mu = A, B),
\]  
(S13)
where \(\phi_{n,A}^{(j)}\) and \(\phi_{n,B}^{(j)}\) takes the exponential form
\[
(\phi_{n,A}^{(j)}, \phi_{n,B}^{(j)}) = \beta^n (\phi_{x,A}^{(j)}, \phi_{x,B}^{(j)}).
\]  
(S14)
By substituting the exponential form Eq. (S14) into Eq. (S12), one can obtain the bulk eigen-equations
\[
\begin{bmatrix}
(t_2 - \frac{\gamma_2}{2}) \beta^{-1} + (t_1 + \frac{\gamma_1}{2}) + t_3 \beta \\
t_3 \beta^{-1} + (t_1 - \frac{\gamma_1}{2}) + (t_2 + \frac{\gamma_2}{2}) \beta
\end{bmatrix} \phi = E \phi,
\]
(S15)
Therefore the characteristic equation can be written as
\[
\left[ \left( t_2 - \frac{\gamma_2}{2} \right) \beta^{-1} + \left( t_1 + \frac{\gamma_1}{2} \right) + t_3 \beta \right] \phi_B = E \phi_A,
\]
\[
\left[ t_3 \beta^{-1} + \left( t_1 - \frac{\gamma_1}{2} \right) + \left( t_2 + \frac{\gamma_2}{2} \right) \beta \right] \phi_A = E \phi_B.
\]
We note that it is the eigenvalue equation for the generalized Bloch Hamiltonian \(H(\beta)\) with \(\beta \equiv e^{i k}, k \in \mathbb{C}\). Henceforth we assume \(t_2 \neq \pm \gamma_2/2\) and \(t_3 \neq 0\), meaning that Eq. (S16) is a quartic equation for \(\beta\), having four solutions \(\beta_j\) \((j = 1, \ldots, 4)\). They are numbered so as to satisfy \(|\beta_1| \leq |\beta_2| \leq |\beta_3| \leq |\beta_4|\).

B. Derivation of the boundary equation and the condition for the continuum bands

First of all, we derive an equation coming from the boundary conditions in our model. In the following, we set the number of unit cells to be \(L\). We write down the boundary condition for \(\psi_{n,\mu}\):
\[
\left( t_1 + \frac{\gamma_1}{2} \right) \psi_{1,B} + t_3 \psi_{2,B} = E \psi_{1,A},
\]
\[
\left( t_1 - \frac{\gamma_1}{2} \right) \psi_{1,A} + \left( t_2 + \frac{\gamma_2}{2} \right) \psi_{2,A} = E \psi_{1,B},
\]
\[
\left( t_2 + \frac{\gamma_2}{2} \right) \psi_{L-1,B} + \left( t_1 + \frac{\gamma_1}{2} \right) \psi_{L,B} = E \psi_{L,A},
\]
\[
t_3 \psi_{L-1,A} + \left( t_1 - \frac{\gamma_1}{2} \right) \psi_{L,A} = E \psi_{L,B}.
\]  
(S17)
Then, by substituting the general solution
\[
\psi_{n,\mu} = \sum_{j=1}^{4} (\beta_j)^n \phi_{x,\mu}^{(j)}, \quad (\mu = A, B)
\]  
(S18)
to Eq. (S17), one can obtain the four equations for the eight coefficients \(\phi_{x,\mu}^{(j)}\) \((j = 1, \ldots, 4, \mu = A, B)\). By recalling that these coefficients satisfy
\[
\phi_{x,\mu}^{(j)} = \frac{E}{(t_2 - \gamma_2/2) \beta_j^{-1} + (t_1 + \gamma_1/2) + t_3 \beta_j} \phi_{x,\mu}^{(j)},
\]
(S19)
from the bulk eigen-equation Eq. (S15), we can reduce the problem into four linear equations for the four coefficients \(\phi_{x,\mu}^{(j)}\) \((j = 1, \ldots, 4)\). Therefore they can be written as
\[
\begin{bmatrix}
1 & 1 & 1 & 1 \\
\beta_1^{-1} & \beta_2^{-1} & \beta_3^{-1} & \beta_4^{-1} \\
X_1 & X_2 & X_3 & X_4 \\
\beta_1^{L} X_1 & \beta_2^{L} X_2 & \beta_3^{L} X_3 & \beta_4^{L} X_4
\end{bmatrix}
\begin{bmatrix}
\phi_{x,1}^{(1)} \\
\phi_{x,2}^{(1)} \\
\phi_{x,3}^{(1)} \\
\phi_{x,4}^{(1)}
\end{bmatrix} = 0,
\]  
(S20)
FIG. S1. Schematic figure of the non-Hermitian SSH model. The system has the asymmetric intracell hopping amplitudes \( t_1 \pm \gamma_1/2 \), the asymmetric nearest-neighbor intercell ones \( t_2 \pm \gamma_2/2 \), and the symmetric next-nearest-neighbor one \( t_3 \). The dotted boxes indicate the unit cell.

where \( X_j \) \( (j = 1, \cdots, 4) \) are defined as

\[
X_j = \frac{1}{(t_2 - \gamma_2/2) \beta_j^{-1} + (t_1 + \gamma_1/2) + t_3 \beta_j}. \tag{S21}
\]

The condition for the determinant of the \( 4 \times 4 \) matrix in Eq. \( \text{(S20)} \) to vanish leads to the boundary equation as

\[
\begin{align*}
&\left[ (\beta_1 \beta_2)^{L+1} + (\beta_3 \beta_4)^{L+1} \right] (X_1 - X_2) (X_3 - X_4) \\
+ &\left[ (\beta_1 \beta_4)^{L+1} + (\beta_2 \beta_3)^{L+1} \right] (X_1 - X_4) (X_2 - X_3) \\
- &\left[ (\beta_1 \beta_3)^{L+1} + (\beta_2 \beta_4)^{L+1} \right] (X_1 - X_3) (X_2 - X_4) = 0.
\end{align*} \tag{S22}
\]

Next we demonstrate that the condition for the continuum bands is given by \( |\beta_2| = |\beta_3| \). We have to consider the condition when the solutions of Eq. \( \text{(S22)} \) are densely distributed for a large \( L \). In the previous work, a simpler case of the characteristic equation being a quadratic equation for \( \beta \) is studied, and the condition for the continuum bands is shown as \( |\beta_i| = |\beta_j| \), i.e., the absolute values of the two solutions being equal. A natural extension of this result \( |\beta_1| = |\beta_2| \) in the case of \( M = 2 \) to a general value of \( M \) is \( |\beta_i| = |\beta_j| \) for some \( i, j \) among the \( 2M \) solutions \( \beta = \beta_j \) \( (j = 1, \cdots, 2M) \). Nevertheless, we find that it is not true.

In the present case of \( M = 2 \), if \( |\beta_2| = |\beta_4| \), the only leading term in Eq. \( \text{(S22)} \) is the term proportional to \( (\beta_3 \beta_4)^{L+1} \), leading to an equation \( (X_1 - X_2)(X_3 - X_4) = 0 \) in the thermodynamic limit \( L \to \infty \). By combining this equation with the characteristic equation \( \text{(S16)} \), the eigenenergies are restricted to discrete values, and it cannot represent continuum bands. On the other hand, if we employ a condition

\[
|\beta_2| = |\beta_3|, \tag{S23}
\]

Eq. \( \text{(S22)} \) has two leading terms, \( (\beta_2 \beta_3)^{L+1} \) and \( (\beta_3 \beta_4)^{L+1} \) for a large \( L \), and Eq. \( \text{(S22)} \) can be rewritten as

\[
\begin{align*}
\left( \frac{\beta_2}{\beta_3} \right)^{L+1} &= \frac{(X_1 - X_2)(X_3 - X_4)}{(X_1 - X_3)(X_2 - X_4)}.
\end{align*} \tag{S24}
\]

For a large \( L \), this equation allows a dense set of solutions when the relative phase between \( \beta_2 \) and \( \beta_3 \) is continuously changed. Therefore we conclude that Eq. \( \text{(S23)} \) is an appropriate condition for the continuum bands. We here emphasize that Eq. \( \text{(S23)} \) is now independent of any boundary conditions. If we change the form of the boundary condition, Eq. \( \text{(S22)} \) may change; nonetheless, Eq. \( \text{(S23)} \) remains the same, and together with the characteristic equation we can obtain the continuum bands.

With a special choice of parameters, the degree of the characteristic equation may become an odd number. For example, when \( t_2 = -\gamma_2/2 \), Eq. \( \text{(S10)} \) becomes a cubic equation for \( \beta \). In this case, we can still regard Eq. \( \text{(S10)} \) as a quartic equation with the limit \( t_2 \to -\gamma_2/2 \) and therefore, by adding another solution \( \beta = \infty \), and our result Eq. \( \text{(S21)} \) holds good with four solutions \( \beta_1, \beta_2, \beta_3, \beta_4(= \infty) \). Thus in general, when the degree of the characteristic equation is odd, one can treat it as a limiting case of an algebraic equation of an even degree, by formally adding a solution \( \beta = 0 \) or \( \beta = \infty \), depending on the system, and the condition for the continuum bands remains valid.

When \( t_3 = 0 \) in our model, the characteristic equation Eq. \( \text{(S16)} \) for \( \beta \) becomes a quadratic equation, and the condition for the continuum bands is \( |\beta_i| = |\beta_j| \), where \( \beta_1 \) and \( \beta_2 \) are two solutions of the characteristic equation. Such cases of quadratic characteristic equations have already been studied in Ref. 1.

C. Generalized Brillouin zone

As an example we show the generalized Brillouin zone \( C_{\beta} \) for parameters \( t_1 = 0.3, t_2 = 0.5, t_3 = 1/5, \gamma_1 = 5/3, \gamma_2 = 1/3 \) in our model. We impose the condition \( |\beta_2| = |\beta_3| \) and calculate the trajectories of \( \beta_2 \) and \( \beta_3 \) shown in Fig. \( \text{S2} \) (a). For comparison we investigate what happens if we impose a condition \( |\beta_i| = |\beta_j| \) for some \( i \) and \( j \) among the four solutions instead. We show the trajectory of \( \beta_1 \) and \( \beta_2 \) in Fig. \( \text{S2} \) (b). In Ref. 1, it was suggested that \( |\beta_i| = |\beta_j| \) is a necessary condition for the continuum bands. Nonetheless, it is not sufficient to get \( C_{\beta} \), and we should restrict this condition to be \( |\beta_2| = |\beta_3| \), leading to \( C_{\beta} \) in Fig. \( \text{S2} \) (a).
In some cases, the generalized Brillouin zone $C_\beta$ can have cusps as seen in Fig. S2(a). It appears when three of the four solutions of $\beta$ share the same absolute value. Suppose $|\beta_1| < |\beta_2| = |\beta_3| < |\beta_4|$, and as we go along $C_\beta$, $|\beta_1|$ approaches $|\beta_2| = |\beta_3|$. Then, when $|\beta_1| = |\beta_2| = |\beta_3|$, the behavior of the solutions satisfying $|\beta_2| = |\beta_3|$ changes, and there appears a cusp in $C_\beta$, as one can compare Figs. S2(a) and (b).

IV. METHODS FOR CALCULATING THE GENERALIZED BRILLOUIN ZONE

We explain the method to get the trajectory of $\beta$ satisfying the continuum-band condition \( S^{23} \). We first express the characteristic equation Eq. \( S^{10} \) as $E^2 = F(\beta)$. Suppose the two solutions $\beta$ and $\beta'$ have the same absolute values: $|\beta| = |\beta'|$. Then we have

$$\beta' = \beta e^{i\theta},$$

where $\theta$ is real. Then, by taking the difference between two equations:

$$E^2 = F(\beta), \quad E^2 = F(\beta e^{i\theta}),$$

we get

$$0 = \left( t_2 - \frac{\gamma_2}{2} \right) t_3 \beta^2 - (1 - e^{-2i\theta})$$

$$+ \left[ \left( t_1 - \frac{\gamma_1}{2} \right) t_3 + \left( t_1 + \frac{\gamma_1}{2} \right) \left( t_2 - \frac{\gamma_2}{2} \right) \right] \beta - (1 - e^{-2i\theta})$$

$$+ \left[ \left( t_1 - \frac{\gamma_1}{2} \right) t_3 + \left( t_1 + \frac{\gamma_1}{2} \right) \left( t_2 + \frac{\gamma_2}{2} \right) \right] \beta - (1 e^{-2i\theta}).$$

This equation allows us to calculate $\beta$ for a given value of $\theta \in (0, 2\pi)$. Then we obtain a set of values of $\beta$ that satisfies $|\beta| = |\beta'|$. Here we should further constrain the values of $\beta$ by Eq. \( S^{22} \). Namely the absolute values of $\beta$ and $\beta'$ should be the second and third largest ones among the four solutions. By selecting the values of $\beta$ and $\beta'$ satisfying this condition, we can get the generalized Brillouin zone.

V. Q MATRIX AND WINDING NUMBER IN 1D NON-HERMITIAN SYSTEMS WITH CHIRAL SYMMETRY

A. Multi-bands model

We focus on 1D non-Hermitian systems with chiral symmetry which have an arbitrary number of bands. In the following, the systems have a gap around $E = 0$, but without exceptional points. Since the systems always have pairs of the eigenenergy $(E, -E)$ due to chiral symmetry, we can assume that the bands are composed of $N$ occupied bands with $E = -E_i$ $(i = 1, \cdots, N)$ and $N$ unoccupied bands with $E = E_i$ $(i = 1, \cdots, N)$. By taking an appropriate basis, the Hamiltonian in the systems can be written as the block off-diagonal form:

$$H(\beta) = \begin{pmatrix} 0 & R_+(\beta) \\ R_-(\beta) & 0 \end{pmatrix},$$

where $\beta = e^{ik}, \ k \in \mathbb{C}$ and $R_{\pm}(\beta)$ are $N \times N$ matrices. The chiral symmetry is expressed as

$$\sigma_z H(\beta) = -H(\beta) \sigma_z, \ \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

where $1$ is an $N \times N$ identity matrix. Then the eigenvalue equations for the right and left eigenstates

$$|\psi_R(\beta)\rangle = \begin{pmatrix} |a_R(\beta)\rangle \\ |b_R(\beta)\rangle \end{pmatrix},$$

$$\langle \psi_L(\beta) | = \left( \langle a_L(\beta) | \langle a_R(\beta) | \right),$$

are given by

$$R_+(\beta) |b_R(\beta)\rangle = E |a_R(\beta)\rangle,$$

$$R_-(\beta) |a_R(\beta)\rangle = E |b_R(\beta)\rangle,$$

respectively. For the right and left eigenstates, one can reduce Eqs. \( S^{21} \) and \( S^{22} \) to

$$R_+(\beta) R_-(\beta) \langle a_R(\beta) | E^2 |a_R(\beta)\rangle = E^2 \langle a_R(\beta) |,$$

$$\langle a_L(\beta) | R_+(\beta) R_-(\beta) = E^2 \langle a_R(\beta) |,$$

respectively. Here we introduce the right and left eigenstates of the $N \times N$ matrix $R_+(\beta) R_-(\beta)$ as $|a_R/L_i(\beta)\rangle, \cdots, |a_R/L_N(\beta)\rangle$, respectively, and the eigenvalues as $E_1^2(\beta), \cdots, E_N^2(\beta)$. Furthermore the right and left eigenstates satisfy

$$\langle a_{L,i}(\beta) | a_{R,j}(\beta) \rangle = \delta_{ij},$$

since one can take the biorthogonal basis $a_{L,i}$. Therefore we can obtain the biorthogonal eigenstates of the Hamiltonian Eq. \( S^{25} \) in the occupied bands for $i = 1, \cdots, N$. 
The right and left eigenstates can be written down as
\[ |\psi_{R,i}(\beta)\rangle = \frac{1}{\sqrt{2}} \left( |a_{R,i}(\beta)\rangle - |a_{L,i}(\beta)\rangle \right), \]
\[ \langle \psi_{L,i}(\beta) | = \frac{1}{\sqrt{2}} \left( |a_{L,i}(\beta)\rangle - |a_{R,i}(\beta)\rangle \right). \]

From Eq. (S42), the Hamiltonian can be written as
\[ \sigma \equiv \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \]
and in the matrix form, it can be written as
\[ Q(\beta) = \sum_{i=1}^{N} \frac{1}{E_i(\beta)} \begin{pmatrix} O & R_- (\beta) |a_{R,i}(\beta)\rangle \langle a_{L,i}(\beta)| \\ R_+ (\beta) |a_{R,i}(\beta)\rangle \langle a_{L,i}(\beta)| & O \end{pmatrix}. \quad (S37) \]

Here we define the matrix \( q(\beta) \) and \( q^{-1}(\beta) \) as
\[ q(\beta) \equiv \sum_{i=1}^{N} \frac{1}{E_i(\beta)} |a_{R,i}(\beta)\rangle \langle a_{L,i}(\beta)| R_+ (\beta), \]
\[ q^{-1}(\beta) = \sum_{i=1}^{N} \frac{1}{E_i(\beta)} R_- (\beta) |a_{R,i}(\beta)\rangle \langle a_{L,i}(\beta)|, \quad (S38) \]
respectively. As a result, one can get the winding number \( w_{\pm} \) as
\[ w = \frac{i}{2\pi} \int_{C_\beta} \text{Tr} \left[ dq q^{-1}(\beta) \right]. \quad (S39) \]

### B. Two-bands model

In particular, we can explicitly write Eq. (S39) in a two-band model. The Hamiltonian can be written as
\[ H(\beta) = R_+ (\beta) \sigma_+ + R_- (\beta) \sigma_- , \quad (S40) \]
where \( \sigma_\pm = (\sigma_x \pm i\sigma_y) / 2 \). Then the eigenvalues are given by
\[ E_\pm(\beta) = \pm \sqrt{R_+ (\beta) R_- (\beta)}. \quad (S41) \]
The right and left eigenstates can be written down as
\[ |u_{R,\pm}\rangle = \frac{1}{\sqrt{2\sqrt{R_+ R_-}}} \left( \frac{R_+}{\sqrt{\pm R_+ R_-}} \right) |a_{R,\pm}(\beta)\rangle, \]
\[ \langle u_{L,\pm}| = \frac{1}{\sqrt{2\sqrt{R_+ R_-}}} \left( R_- \pm \sqrt{R_+ R_-} \right), \quad (S42) \]
respectively. The subscript \(+/-\) means that the eigenstates with \(+/-\) have the eigenvalues \( E_+ \) or \( E_- \), respectively. From Eq. (S42), the \( Q \) matrix \( Q(\beta) \) can be written down by
\[ Q(\beta) = |u_{R,\pm}(\beta)\rangle \langle u_{L,\pm}(\beta)| - |u_{R,\pm}(\beta)\rangle \langle u_{L,\pm}(\beta)| \]
\[ = \frac{1}{\sqrt{R_+ (\beta) R_- (\beta)}} \begin{pmatrix} 0 & R_+ (\beta) \\ R_- (\beta) & 0 \end{pmatrix}. \quad (S43) \]

Then the unoccupied eigenstates are given by
\[ |\psi_{R/L,i}(\beta)\rangle \equiv \sigma_\pm |\psi_{R/L,i}(\beta)\rangle. \]
In the systems, the \( Q \) matrix \( Q(\beta) \) can be defined as
\[ Q(\beta) = \sum_{i=1}^{N} \left( |\psi_{R,i}(\beta)\rangle \langle \psi_{L,i}(\beta)| - |\psi_{R,i}(\beta)\rangle \langle \psi_{L,i}(\beta)| \right) \]
and in the matrix form, it can be written as
\[ \begin{pmatrix} |a_{R,i}(\beta)\rangle \langle a_{L,i}(\beta)| R_+ (\beta) \\ O \end{pmatrix}. \quad (S37) \]

Therefore we can obtain \( q = R_+ / \sqrt{R_+ R_-} \), and the winding number \( w \) explicitly as
\[ w = \frac{i}{2\pi} \int_{C_\beta} dq q^{-1}(\beta) = \frac{i}{2\pi} \int_{C_\beta} d\log q(\beta) = -\frac{1}{2\pi} [\arg R_+ (\beta) - \arg R_- (\beta)]_{C_\beta}. \quad (S44) \]

Thus the winding number \( w \) is determined by the change of the phase of \( R_\pm(\beta) \) when \( \beta \) goes along the generalized Brillouin zone \( C_\beta \). On a complex plane, let \( \ell_\pm \) denote the loops drawn by \( R_\pm(\beta) \) when \( \beta \) goes along \( C_\beta \) in the counterclockwise way. Then \( w \) is determined by the number of times that \( \ell_\pm \) surround the origin \( O \). When neither \( \ell_+ \) nor \( \ell_- \) surround \( O \), \( w \) is zero. It takes a non-zero value when they simultaneously surround \( O \).

Here we can show the bulk-edge correspondence in this case. If parameters of the system can be continuously changed without closing the gap, the winding number \( w \) does not change, and the topology of the systems remains invariant. Namely, if the systems after changing the values of the parameters have the zero-energy edge states, one can conclude that the original systems also have the zero-energy edge states. This can be proved even in non-Hermitian cases, following the proof in Hermitian systems.

Suppose we change the parameters of the system continuously, and at some values of the parameters \( \ell_+ \) and \( \ell_- \) simultaneously pass the origin \( O \) on the \( R \) plane. At this time, the gap closing occurs because the energy eigenvalues are given by Eq. (S41).

In Hermitian systems, \( R_+^* = R_- \) holds, and two loops \( \ell_+ \) and \( \ell_- \) are related by complex conjugation, so
\[ [\arg R_- (\beta)]_{C_\beta} = -[\arg R_+ (\beta)]_{C_\beta}. \quad (S45) \]
In contrast with these cases, in some non-Hermitian systems, only one of the two loops \( \ell_+ \) and \( \ell_- \) passes the
VI. CALCULATION ON ANOTHER MODEL

We investigate the non-Hermitian tight-binding model proposed in Ref. [6] as shown in Fig. S3. The previous work proposed that anomalous edge states, which are localized at the either end of a finite open chain appear in this model. In this supplemental material, we reveal that this model corresponds to the non-Hermitian SSH model as shown in Fig. S4 with \( t_3 = \gamma_2 = 0 \).

First of all, we can write the Hamiltonian in this model as

\[
H = \sum_n \left[ v \left( c_{n,+}^\dagger c_{n,-} + c_{n,-}^\dagger c_{n,+} \right) + \frac{ir}{2} \left( c_{n+1,+}^\dagger c_{n,-} - c_{n,-}^\dagger c_{n+1,+} - c_{n+1,-}^\dagger c_{n,+} + c_{n,+}^\dagger c_{n+1,-} \right) + \frac{r}{2} \left( c_{n+1,+}^\dagger c_{n,-} + c_{n,-}^\dagger c_{n+1,+} + c_{n+1,-}^\dagger c_{n,+} + c_{n,+}^\dagger c_{n+1,-} \right) \right],
\]

where we take \( r, v, \) and \( \gamma \) to be real for simplicity. When the eigenvector of the real-space eigen-equation is written as \( \psi = (\psi_{1,\alpha}, \psi_{1,\beta}, \cdots, \psi_{L,\alpha}, \psi_{L,\beta})^T \) in an open chain, the equation for \( \psi_{n,\mu} \) can be written as

\[
\frac{ir}{2} \left( \psi_{n-1,\alpha} - \psi_{n+1,\alpha} \right) + \frac{r}{2} \left( \psi_{n-1,\beta} + \psi_{n+1,\beta} \right) + v \psi_{n,\beta} = E \psi_{n,\alpha},
\]

\[
\frac{ir}{2} \left( \psi_{n-1,\beta} - \psi_{n+1,\beta} \right) - \frac{r}{2} \psi_{n,\beta} = E \psi_{n,\alpha}
\]

\[
+ \frac{r}{2} \left( \psi_{n-1,\alpha} + \psi_{n+1,\alpha} \right) + v \psi_{n,\alpha} = E \psi_{n,\beta}. \tag{S47}
\]

Here we take the ansatz as a linear combination:

\[
\psi_{n,\mu} = \sum_j \phi_{n,\mu}^{(j)}, \quad \phi_{n,\mu}^{(j)} = (\beta_j)^n \phi_j^{(\mu)}, \quad (\mu = \alpha, \beta), \tag{S48}
\]

where \( \phi_{n,\alpha}^{(j)} \) and \( \phi_{n,\beta}^{(j)} \) take the exponential form

\[
\left( \phi_{n,\alpha}^{(j)}, \phi_{n,\beta}^{(j)} \right) = \beta_j^n \left( \phi_\alpha^{(j)}, \phi_\beta^{(j)} \right). \tag{S49}
\]

By substituting the exponential form Eq. \( \text{S49} \) into Eq. \( \text{S47} \), one can obtain

\[
\left[ -\frac{ir}{2} (\beta - \beta^{-1}) + \frac{r}{2} \right] \phi_\alpha + \left[ \frac{r}{2} (\beta + \beta^{-1}) + v \right] \phi_\beta = E \phi_\alpha,
\]

\[
\left[ \frac{ir}{2} (\beta - \beta^{-1}) - \frac{r}{2} \right] \phi_\beta + \left[ \frac{r}{2} (\beta + \beta^{-1}) + v \right] \phi_\alpha = E \phi_\beta. \tag{S50}
\]

Therefore the characteristic equation is given by

\[
r \left( v + \frac{\gamma}{2} \right) \beta + \left( r^2 + v^2 - \frac{\gamma^2}{4} - E^2 \right) + \frac{r}{2} \left( v - \frac{\gamma}{2} \right) \beta^{-1} = 0. \tag{S51}
\]

The condition for the continuum bands can be written as \( |\beta_1| = |\beta_2| \) since Eq. \( \text{S51} \) is a quadratic equation for \( \beta \). In this case, the generalized Brillouin zone becomes a circle with the radius

\[
r = |\beta_{1,2}| = \sqrt{\frac{v - \gamma/2}{v + \gamma/2}} \tag{S52}
\]

which is given by Vieta’s formula. By substituting \( \beta = re^{i\theta}, \ k \in \mathbb{R} \) to Eq. \( \text{S51} \), we can get the gap-closing point as

\[
\frac{v}{\gamma} = \pm \sqrt{\frac{1}{4} \pm \left( \frac{r}{\gamma} \right)^2}. \tag{S53}
\]

Therefore the zero-energy edge states appear in the parameter region \( v/\gamma \in \left[ -\frac{\sqrt{1/4 + \left( r/\gamma \right)^2}}, \frac{\sqrt{1/4 - \left( r/\gamma \right)^2}} \right] \) and \( v/\gamma \in \left[ -\frac{\sqrt{1/4 - \left( r/\gamma \right)^2}}, \frac{\sqrt{1/4 + \left( r/\gamma \right)^2}} \right] \) as a consequence of the previous discussion. Indeed, we confirm the appearance of these zero-energy edge states in a finite open chain with \( v/\gamma = 0.5 \). The gap closes at
FIG. S4. Energy bands in a finite open chain of the model given by Eq. (S46). We set the parameter as $r = 0.5\gamma$ and the number of unit cells as $L = 50$. The gap closes at $v/\gamma = 0$ and $v/\gamma = \pm c = \pm 1/\sqrt{2}$. The red dashed lines represent the gap-closing points in the bulk.

The tight-binding model in Fig. S3 can be regarded as the non-Hermitian SSH model. Indeed, by the unitary transformation

$$\sigma_x \rightarrow \sigma_x, \quad \sigma_y \rightarrow -\sigma_z, \quad \sigma_z \rightarrow \sigma_y,$$

the generalized Bloch Hamiltonian $H(\beta)$ can be rewritten as

$$H(\beta) = \left[ v + \frac{r}{2}(\beta + \beta^{-1}) \right] \sigma_x + \left[ \frac{-ir}{2}(\beta - \beta^{-1}) + \frac{i\gamma}{2} \right] \sigma_z$$

$$\rightarrow \left( v + \frac{\gamma}{2} + r\beta^{-1} \right) \sigma_+ + \left( v - \frac{\gamma}{2} + r\beta \right) \sigma_-,$$

where $\sigma_\pm = (\sigma_x \pm i\sigma_y)/2$. We note that the asymmetric hopping amplitude is caused by the gain and loss in the original system. This Hamiltonian is reduced to our model with $t_3 = \gamma_2 = 0$.

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