Edge states and topological invariants of non-Hermitian systems

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The bulk-boundary correspondence is among the central issues of non-Hermitian topological states. We show that a previously overlooked “non-Hermitian skin effect” necessitates redefinition of topological invariants in a generalized Brillouin zone. The resultant phase diagrams dramatically differ from the usual Bloch theory. Specifically, we obtain the phase diagram of non-Hermitian Su-Schrieffer-Heeger model, whose topological zero modes are determined by the non-Bloch winding number instead of the Bloch-Hamiltonian-based topological number. Our work settles the issue of the breakdown of conventional bulk-boundary correspondence and introduces the non-Bloch bulk-boundary correspondence.

**Introduction.**—Topological materials are characterized by robust boundary states immune to perturbations$^{[1-5]}$. According to the principle of bulk-boundary correspondence, the existence of boundary states is dictated by the bulk topological invariants, which, in the band-theory framework, are defined in terms of the Bloch Hamiltonian. The Hamiltonian is often assumed to be Hermitian. In many physical systems, however, non-Hermitian Hamiltonians are more appropriate$^{[6,7]}$. For example, they are widely used in describing open systems$^{[8-17]}$, wave systems with gain and loss$^{[18-40]}$ (e.g. photonic and acoustic$^{[41-44]}$), and solid-state systems where electron-electron interactions or disorders introduce a non-Hermitian self energy into the effective Hamiltonian of quasiparticles$^{[45-47]}$. With these physical motivations, there have recently been growing efforts, both theoretically$^{[48-78]}$ and experimentally$^{[79-85]}$, to investigate topological phenomena of non-Hermitian Hamiltonians.

Among the key issues is the fate of bulk-boundary correspondence in non-Hermitian systems. Recently, numerical results in a one-dimensional (1D) model show that open-boundary spectra look notably different from periodic-boundary ones, which seems to indicate a complete breakdown of bulk-boundary correspondence$^{[49,86]}$. In view of this breakdown, a possible scenario is that the topological edge states depend on all sample details, without any general rule telling their existence or absence. Here, we ask the following questions: Is there a generalized bulk-boundary correspondence? Are there bulk topological invariants responsible for the topological edge states? Affirmative answers are obtained in this paper.

We start from solving a 1D model. Interestingly, all the eigenstates of an open chain are found to be localized near the boundary (dubbed “non-Hermitian skin effect”), in contrast to the extended Bloch waves in Hermitian cases. In the simplest situations, this effect can be understood in terms of an imaginary gauge field$^{[87,88]}$. We show that the non-Hermitian skin effect has dramatic consequences in establishing a “non-Bloch bulk-boundary correspondence” in which the topological boundary modes are determined by “non-Bloch topological invariants”.

Previous non-Hermitian topological invariants$^{[48-56]}$ are formulated in terms of the Bloch Hamiltonian. The crucial non-Bloch-wave nature of eigenstates (non-Hermitian skin effect) is untouched, therefore, the number of topological edge modes is not generally related to these topological invariants. In view of the non-Hermitian skin effect, we introduce a non-Bloch topological invariant, which faithfully determines the number of topological edge modes. It embodies the non-Bloch bulk-boundary correspondence of non-Hermitian systems.

**Model.**—The non-Hermitian Su-Schrieffer-Heeger (SSH) model$^{[85,90]}$ is pictorially shown in Fig.1. Related models are relevant to quite a few experiments$^{[79,82,91]}$. The Bloch Hamiltonian is

\[
H(k) = d_x \sigma_x + (d_y + i \gamma/2) \sigma_y,
\]

where $d_x = t_1 + (t_2 + t_3) \cos k$, $d_y = (t_2 - t_3) \sin k$, and $\sigma_{xy}$ are the Pauli matrices. A mathematically equivalent model was studied in Ref. [49], where $\sigma_y$ was replaced by $\sigma_z$; as such, the physical interpretation was not SSH. The model has a chiral symmetry [3]: $\sigma_z^{-1} H(k) \sigma_z = -H(k)$, which ensures that the eigenvalues appear in $(E, -E)$ pairs: $E_\pm(k) = \pm \sqrt{d_x^2 + (d_y + i \gamma/2)^2}$. Let us first take $t_2 = 0$ for simplicity (nonzero $t_2$ will be included later). The energy gap closes at the exceptional points $(d_x, d_y) = (\pm \gamma/2, 0)$, which requires $t_1 = t_2 = \gamma/2$ ($k = \pi$) or $t_1 = -t_2 = \gamma/2$ ($k = 0$).

The open-boundary spectrum is noticeably different from that of periodic boundary$^{[49,92]}$, which can be seen in the numerical spectra of real-space Hamiltonian of an open chain [Fig.2]. The zero modes are robust to perturbation [Fig.2(d)], which indicates their topological origin. A transition point is located at $t_1 \approx 1.20$, which is a quite unremarkable point from the perspective of $H(k)$ whose spectrum is gapped there ($|E_\pm(k)| \neq 0$). As such, the topology of $H(k)$ cannot determine the zero modes, which challenges the familiar Hermitian wis-
We can judiciously choose $S$ in this similarity transformation. Let us take $S$ to be a diagonal matrix whose diagonal elements are $\{1, r, r, r^2, \ldots, r^{L-1}, r^L\}$, then in $\hat{H}$ we have $r^{1}(t_1 + \gamma/2)$ in the place of $t_1 \pm \gamma/2$ (Fig.[1]). If we take $r = \sqrt{t_1/(t_1 + \gamma/2)}$, $\hat{H}$ becomes the standard SSH model for $|t_1| > |\gamma/2|$, with intracell and intercell hoppings
\[
\tilde{t}_1 = \sqrt{(t_1 - \gamma/2)(t_1 + \gamma/2)}, \quad \tilde{t}_2 = t_2.
\] (3)

The $k$-space expression is
\[
\hat{H}(k) = (\tilde{t}_1 + \tilde{t}_2 \cos k)\sigma_x + \tilde{t}_2 \sin k\sigma_y.
\] (4)

The transition points are $\tilde{t}_1 = \tilde{t}_2$, namely
\[
t_1 = \pm \sqrt{t_0^2 + (\gamma/2)^2}.
\] (5)

For the parameters in Fig[2], Eq. (5) gives $t_1 \approx \pm 1.20$. Note that any $H(k)$-based topological invariants[16,51] can jump only at $t_1 = \pm t_2 + \gamma/2$, where the gap of $H(k)$ closes.

A bulk eigenstate $|\psi_j\rangle$ of Hermitian $\hat{H}$ is extended, therefore, $H$'s eigenstate $|\psi_j\rangle = \hat{S}|\tilde{\psi}_j\rangle$ is exponentially localized at an end of the chain when $\gamma \neq 0$. It implies that the usual Bloch phase factor $e^{ik}$ is replaced by $\beta = e^{ik}$ in the open-boundary system (i.e., the wavevector acquires an imaginary part: $k \to k - i \ln |r|$). Although this intuitive picture is based on the shortcut solution, we believe that the exponential-decay behavior of eigenstates (“non-Hermitian skin effect”) is a general feature of non-Hermitian bands.

Generalizable solution.—The intuitive shortcut solution has limitations: e.g., it is inapplicable when $t_1 \neq 0$. Here, we re-derive the solution in a more generalizable way (still focusing on $t_3 = 0$ for simplicity). The real-space eigen-equation leads to $t_2|\psi_{n+1,B} = (t_1 + \frac{\gamma}{2})|\psi_{n,B} = E|\psi_{n,A}\rangle$ and $(t_1 - \frac{\gamma}{2})|\psi_{n,B} = E|\psi_{n,A}\rangle$ in the bulk of chain. We take the ansatz that $|\psi\rangle = \sum_j |\phi_j\rangle$, where each $|\phi_j\rangle$ takes the exponential form (omitting the $j$ index temporarily): $|\phi_j\rangle = \beta^j|\phi_A, \phi_B\rangle$, which satisfies
\[
[(t_1 + \frac{\gamma}{2}) + t_2\beta^{-1}]|\phi_B = E|\phi_A, [(t_1 - \frac{\gamma}{2}) + t_2\beta]|\phi_A = E|\phi_B. (6)
\]

Therefore, we have
\[
[(t_1 - \frac{\gamma}{2}) + t_2\beta][(t_1 + \frac{\gamma}{2}) + t_2\beta^{-1}] = E^2.
\] (7)

which has two solutions, namely $\beta_{1,2}(E) = \frac{E^2 + \gamma^2/4 - \epsilon^2}{2i t_2(t_1 + \gamma/2)}, \frac{E^2 + \gamma^2/4 - \epsilon^2}{2i t_2(t_1 + \gamma/2)}$, where $(\pm)$ corresponds to $\beta_1, \beta_2$. In the $E \to 0$ limit, we have
\[
\beta_{1,2}^{E=0} = \frac{-t_1 - \gamma/2}{t_2}, \frac{-t_2}{t_1 + \gamma/2}.
\] (8)

They can also be seen from Eq.(6). These two solutions correspond to $\phi_B = 0$ and $\phi_A = 0$, respectively.

Restoring the $j$ index in $|\phi_j\rangle$, we have
\[
|\phi_A^j\rangle = \frac{E}{t_1 - \gamma/2 + t_2\beta_j} |\phi_A^{(1)}j\rangle, \quad |\phi_B^j\rangle = \frac{E}{t_1 + \gamma/2 + t_2\beta_j} |\phi_B^{(2)}j\rangle.
\] (9)

These two equations are equivalent because of Eq.(7). The general solution is written as a linear combination:
\[
|\psi_{n,A}\rangle = \beta_1^{(1)}|\phi_A^{(1)}j\rangle + \beta_2^{(2)}|\phi_A^{(2)}j\rangle.
\] (10)
which should satisfy the boundary condition

\[(t_1 + \gamma/2)\psi_{1,B} - E\psi_{1,A} = 0, \quad (t_1 - \gamma/2)\psi_{L,A} - E\psi_{L,B} = 0.\]  

Together with Eq. (9), they lead to

\[\beta_1^{l+1}(t_1 - \gamma/2 + t_2\beta_2) = \beta_2^{l+1}(t_1 + \gamma/2 + t_2\beta_1).\]  

We are concerned about the spectrum for a long chain, which necessitates \(|\beta_1| = |\beta_2|\) for the bulk eigenstates. If not, suppose that \(|\beta_1| < |\beta_2|\), we would be able to discard the tiny \(\beta_1^{l+1}\) term in Eq. (12), and the equation becomes \(\beta_2 = 0\) or \(t_1 - \gamma/2 + t_2\beta_1 = 0\) (without the appearance of \(L\)). As a bulk-band property, \(|\beta_1(E)| = |\beta_2(E)|\) remains valid in the presence of perturbations near the edges [e.g., Fig. 2(d)], and essentially determines the bulk-band energies \(|\beta_2|\). Combined with \(\beta_1\beta_2 = \frac{t_1 - \gamma/2}{t_1 + \gamma/2}\) coming from Eq. (7), \(|\beta_1| = |\beta_2|\) leads to

\[|\beta_j| = r \equiv \sqrt{\frac{t_1 - \gamma/2}{t_1 + \gamma/2}}\]  

for bulk eigenstates (i.e., eigenstates in the continuum spectrum). The same \(r\) has just been used in the shortcut solution.

We emphasize that \(r < 1\) indicates that all the eigenstates are localized at the left end of the chain [see Fig. 3(c) for illustration]. In Hermitian systems, the orthogonality of eigenstates excludes this "non-Hermitian skin effect".

There are various ways to re-derive the transition points in Eq. (5). To introduce one of them, we first plot in Fig. 3(a) the \(|\beta_j|\)-E curve solved from Eq. (7) for \(t_1 = t_2 = 1, \gamma = 4/3\). The spectrum is real for this set of parameters, therefore, no imaginary part of \(E\) is needed (This reality is related to PT symmetry\(^{(5)}\)). The expected \(|\beta_1| = |\beta_2| = r\) relation is found on the line \(FG\) (Fig. 3(a)), which is associated with bulk spectra. As \(t_1\) is increased from 1, \(F\) moves towards left, and finally hits the \(|\beta|\) axis (\(E = 0\) axis). Apparently, it occurs when \(|\beta_1^{E=0}| = |\beta_2^{E=0}| = r\). Inserting Eq. (8) into this equation, we have

\[t_1 = \pm \sqrt{t_2^2 + (\gamma/2)^2} \quad \text{or} \quad \pm \sqrt{-t_2^2 + (\gamma/2)^2}.\]  

At these points, the open-boundary continuum spectra touch zero energy, enabling topological transitions. A simpler way to re-derive Eq. (5) is to calculate the open-boundary spectra. According to Eq. (13), we can take \(\beta = re^{ik}\) \((k \in [0, 2\pi])\) in Eq. (7) to obtain the spectra:

\[E^2(k) = t_1^2 + t_2^2 - \gamma^2/4 + t_2 \sqrt{(t_1^2 - \gamma^2/4)(\text{sgn}(t_1 + \gamma/2)e^{ik}) + \text{sgn}(t_1 - \gamma/2)e^{-ik})},\]  

which recovers the spectrum of SSH model when \(\gamma = 0\). The spectral are real when \(t_1 > |\gamma|/2\). Eq. (14) can be readily re-derived as the gap-closing condition of Eq. (15) \((E(k) = 0)\).

Before proceeding, we comment on a subtle issue in the standard method of finding zero modes. For concreteness, let us consider the present model, and focus on zero modes at the left end of a long chain. One can see that \(\psi_{\text{zero}}\) with \((\psi_{\text{zero}}) = (\beta_1^{E=0}f(1, 0))\) appears as a zero-energy eigenstate (see Eq. (8) for \(\beta_1^{E=0}\)). In the standard approach, the normalizable condition \(|\beta_1^{E=0}| < 1\) is imposed, and the transition points satisfy \(|\beta_1^{E=0}| = 1\), which predicts \(t_1 = t_2 + \gamma/2\) as a transition point, being consistent with the gap closing of \(H(k)\). Such an apparent but misleading consistency has hidden the true transition points and topological invariants in quite a few previous studies of non-Hermitian models. The implicit assumption was that the bulk eigenstates are extended Bloch waves with \(|\beta| = 1\), into which the zero modes merge at transitions. In reality, the bulk eigenstates have \(|\beta| = r\) (eigenstate skin effect); therefore, the true merging-into-bulk condition is

\[|\beta_1^{E=0}| = r,\]  

which correctly produces \(t_1 = \sqrt{t_2^2 + (\gamma/2)^2}\). This is a manifestation of the non-Bloch bulk-boundary correspondence.

Non-Bloch topological invariant. The bulk-boundary correspondence is fulfilled if we can find a bulk topological invariant that determines the edge modes. Previous constructions take \(H(k)\) as the starting point\(^{(48, 50)}\), which should be revised in view of the non-Hermitian skin effect. The usual Bloch waves carry a pure phase factor \(e^{ik}\), whose role is now
played by $\beta$. In addition to the phase factor, $\beta$ has a modulus $|\beta| \neq 1$ in general [e.g., Eq. (13)]. Therefore, we start from the “non-Bloch Hamiltonian” obtained from $H(k)$ by the replacement $e^{ik} \rightarrow e^{-i\beta k}$:

$$H(\beta) = (t_1 - \gamma/2 + \beta t_2)\sigma_z + \left(1 + \gamma/2 + \beta^{-1} t_2\right)\sigma_+,$$

where $\sigma_\pm = (\sigma_z \pm i\sigma_x)/2$. We have taken $t_3 = 0$ for simplicity. As explained in both the shortcut and generalizable solutions, $\beta$ takes values in a non-unit circle $|\beta| = r$ (in other words, $k$ acquires an imaginary part $-i\ln r$). It is notable that the open-boundary spectra in Eq. (15) are given by $H(\beta)$ instead of $H(k)$.

The right and left eigenvectors are defined by

$$H(\beta)|u_k\rangle = E(\beta)|u_k\rangle, \quad H^\dagger(\beta)|u_{-k}\rangle = E^\ast(\beta)|u_{-k}\rangle.$$

Chiral symmetry ensures that $|u_{R}\rangle \equiv \sigma_z|u_L\rangle$ and $|\tilde{u}_L\rangle \equiv \sigma_z|u_R\rangle$ is also right and left eigenvector, with eigenvalues $-E$ and $-E^\ast$, respectively. In fact, one can diagonalize the matrix as $H(\beta) = TJT^{-1}$ with $J = \begin{pmatrix} 0 & E \\ -E & 0 \end{pmatrix}$, then each column of $T$ and $(T^{-1})^\dagger$ is a right and left eigenvector, respectively, and the normalization condition $\langle u_{l}\rangle|u_k\rangle = \langle \tilde{u}_{l}\rangle|\tilde{u}_k\rangle = 1, \langle u_{l}\rangle|\tilde{u}_k\rangle = \langle \tilde{u}_{l}\rangle|u_k\rangle = 0$ is guaranteed. As a generalization of the usual “$Q$ matrix” [3], we define

$$Q(\beta) = |\tilde{u}_R(\beta)\rangle\langle \tilde{u}_L(\beta)| - |u_R(\beta)\rangle\langle u_L(\beta)|,$$

which is off-diagonal due to the chiral symmetry $\sigma^{-1}_z Q \sigma_z = -Q$, namely $Q = \begin{pmatrix} q_1 & q_2 \\ q_2^\ast & q_1^\ast \end{pmatrix}$. Now we introduce the non-Bloch winding number:

$$W = \frac{i}{2\pi} \int_{C_\beta} q^1 dq.$$

Crucially, it is defined on the “generalized Brillouin zone” $C_\beta$ [Fig. 3b]. It is useful to mention that the conventional formulations using $H(k)$ may sometimes produce correct phase diagrams, if $C_\beta$ happens to be a unit circle [92].

The numerical results for $t_3 = 0$ is shown in Fig. 5 which is consistent with the analytical spectra obtained above. Quantitatively, $2W$ counts the total number of robust zero modes at the left and right ends. For example, corresponding to Fig. 2 there are two zero modes for $t_1 \in [-\sqrt{t_2^2 + (\gamma/2)^2}, \sqrt{t_2^2 + (\gamma/2)^2}]$, and none elsewhere. The analytic solution shows that, for $[t_2 - \gamma/2, \sqrt{t_2^2 + (\gamma/2)^2}]$, both modes live at the left end; for $[-t_2 + \gamma/2, t_2 - \gamma/2]$, one for each end; and for $[-\sqrt{t_2^2 + (\gamma/2)^2}, -t_2 + \gamma/2]$, both at the right end. Thus, the $H(\beta)$-gap closing points $\pm(t_2 - \gamma/2)$ are where zero modes migrate from one end to the other, conserving the total mode number. In fact, one can see $|Q|_{j=1,2} = 1$ at $\pm(t_2 - \gamma/2)$, indicating the penetration into bulk.

To provide a more generic exemplification, we take a nonzero $t_3$. Now we find [93] that $C_\beta$ is no longer a circle (bulk eigenstates with different energies have different $\beta$), yet $2W$ correctly predicts the total zero-mode number (Fig. 5).

Finally, we remarked that Eq. (20) can be generalized to multi-band systems. Each pair of bands (labeled by $l$) possesses a $C_{\beta l}^0$ curve, and the $Q$ matrix [Eq. (19)] becomes $Q^0$, each one defining a winding number $W_{l0}$ (with matrix trace). The topological invariant is $W = \sum_l W_{l0}$.

**Conclusions.**—Through the analytic solution of non-Hermitian SSH model, we explained why the usual bulk-boundary correspondence breaks down, and how the non-Bloch bulk-boundary correspondence takes its place. Two of the key concepts are the non-Hermitian skin effect and generalized Brillouin zone. We formulate the generalized bulk-boundary correspondence by introducing a precise topological...
invariant that faithfully predicts the topological edge modes. The physics presented here can be generalized to a rich variety of non-Hermitian systems, which will be left for future studies.

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[93] Supplemental Material.

[94] Recently we noticed Ref. 98, in which similar localization is found numerically; however, in contrast to our viewpoint, it is suggested there that the localization lessens the relevance of zero modes and destroys bulk-boundary correspondence. Also note that the zero-mode interval in their Fig.1 differs from our exact solutions.

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Supplemental Material

Two supplemental figures.—As explained in the main article, the equation \(|\beta_1(E)| = |\beta_2(E)|\) determines the bulk-band energies [see the discussion below Eq. (12) in the main article]. In fact, in the complex \(E\) plane, \(|\beta_1(E)| = |\beta_2(E)|\) determines one-dimensional curves containing the bulk-band energies. Fig. 6 illustrates calculating bulk-band energies by solving \(|\beta_1(E)| = |\beta_2(E)|\) for three values of \(t_1\).

Fig. 7 shows the energies and topological invariant for the parameter regime \(|t_2| < |\gamma/2|\) (In the main article, we have focused on \(|t_2| > |\gamma/2|\)).

Nonzero \(t_3\).—Let us outline the calculation of generalized Brillouin zone \(C_\beta\) for nonzero \(t_3\). We consider an open-boundary chain with length \(L\). In the bulk, the real-space eigen-equations are

\[
\begin{align*}
\mathbf{t}_2 \psi_{n-1, B} + \left( t_1 + \frac{\gamma}{2} \right) \psi_{n, B} + \mathbf{t}_3 \psi_{n+1, B} &= \mathbf{E} \psi_{n, A} \\
\mathbf{t}_3 \psi_{n-1, A} + \left( t_1 - \frac{\gamma}{2} \right) \psi_{n, A} + \mathbf{t}_2 \psi_{n+1, A} &= \mathbf{E} \psi_{n, B}
\end{align*}
\]

Similar to Eq. (21), we now have

\[
\begin{align*}
|t_2\beta_1^{-1} + (t_1 + \frac{\gamma}{2}) + t_3\beta_1| \phi_B &= E\phi_A, \\
|t_3\beta_1^{-1} + (t_1 - \frac{\gamma}{2}) + t_2\beta_1| \phi_A &= E\phi_B.
\end{align*}
\]

Therefore, \(\beta\) and \(E\) satisfy

\[
E^2 = |t_2\beta_1^{-1} + (t_1 + \gamma/2) + t_3\beta_1| |t_1\beta_1^{-1} + (t_1 - \gamma/2) + t_2\beta_1|.
\]

As a quartic equation of \(\beta\), it has four roots \(\beta_j(E)\) \((j = 1, 2, 3, 4)\). As explained in the main article, the bulk-band energies have to satisfy \(||\beta_j(E)| = |\beta_j(E)|\) for a pair of \(i, j\). In fact, this equation can also be intuitively understood as follows. Suppose that a wave with \(\beta_i\) propagates from the left end towards the right. It hits the right end and gets reflected, and the reflected waves with \(\beta_j\) propagates back to the left end. To satisfy certain standing-wave conditions for an energy eigenstate, the magnitudes of the initial and the final waves have to be of the same order, therefore, one must have \(|\beta_1(E)|^2 = |\beta_3(E)|^2\) or \(|\beta_2(E)| = |\beta_4(E)|\). Each equation \(|\beta_j(E)| = |\beta_j(E)|\) determines a one-dimensional curve in the complex \(E\) plane, and the \(\beta\) curve follows from the \(E\) curves.

There is also a more brute-force approach to find the \(C_\beta\) curve. One can numerically solve the eigen-energies of an
open chain, and then find $\beta_j(E)$'s from Eq. (22). In this calculations, one has to discard $\beta_i(E), \beta_j(E)$ that do not satisfy $|\beta_i(E)| = |\beta_j(E)|$, as they should not be regarded as bulk components of the eigenstates. This disposal is similar to the Hermitian case: A typical eigenstate of an open chain is a superposition of right-propagating and left-propagating Bloch waves (both have $|\beta| = 1$) and certain decaying components localized at the two ends. The (Hermitian) topological invariants are defined in terms of the bulk components, namely the Bloch waves.