Defective Edge States and Anomalous Bulk-Boundary Correspondence in non-Hermitian Topological Systems

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Non-Hermitian topological systems show quite different properties as their Hermitian counterparts. An important, puzzled issue on non-Hermitian topological systems is the existence of defective edge states beyond usual bulk-boundary correspondence (BBC) that localize either on the left edge or the right edge of the one-dimensional system. In this paper, to understand the existence of the defective edge states, the theory of anomalous bulk-boundary correspondence (A-BBC) is developed that distinguishes the non-Bloch bulk-boundary correspondence (NB-BBC) from non-Hermitian skin effect. By using the one-dimensional non-Hermitian Su-Schrieffer-Heeger model as an example, the underlying physics of defective edge states is explored. The defective edge states are physics consequence of boundary exceptional points of anomalous edge Hamiltonian. In addition, with the help of a theorem, the number anomaly of the edge states in non-Hermitian topological systems becomes a mathematic problem under quantitative calculations by identifying the Abelian/non-Abelian non-Hermitian condition for edge Hamiltonian and verifying the deviation of the BBC ratio from 1. In the future, the theory for A-BBC can be generalized to higher dimensional non-Hermitian topological systems (for example, 2D Chern insulator).

Introduction to non-Hermitian topological systems: Topological systems, including topological insulators and topological superconductors are new types of exotic quantum phases of matter that have become the forefront of condensed matter physics for many years1–5. An important topological property for different types of topological systems is bulk-boundary correspondence (BBC), i.e., bulk topological invariants that characterize the topological systems correspond to unique gapless boundary (edge) states. Recently, non-Hermitian (NH) topological systems have been intensively studied in both theory6–43 and experiments44–52. The topological properties of NH systems are quite different with their Hermitian counterparts, including the fractional topological invariant and defective edge states11,22, the breakdown of traditional BBC16,19–21,35–37,39,42, and NH skin effect19,29,40,42, and so on. Recently, within the framework of Altland-Zirnbauer (AZ) theory, the classification of NH systems with topological bands is characterized by different symmetry-protected topological invariants18,31,52.

Puzzle about defective edge states: An important, puzzled issue on NH topological systems is the existence of defective edge states (DESs) beyond usual BBC. The DES is a zero mode localized either on the left edge or the right edge of a one-dimensional (1D) finite NH topological system that is firstly discovered numerically by Lee in 2016. In Ref.11, Lee pointed out that it is the fractional winding number that guarantees the DESs and a new type of BBC exists. However, due to the existence of non-Hermitian skin effect, the fractional winding number corresponding to DESs fails. In Ref.19, Yao and Wang pointed out that it is non-Bloch topological invariants rather than fractional winding number that characterize the topological properties of the NH topological system. The energy spectra of the NH topological system under open boundary condition (OPB) may differ from those under periodic boundary condition (PBC). The new BBC is called non-Bloch BBC or NB-BBC for short. With the help of NB-BBC, people can obtain the correct topological phase diagram and know the condition whether the edge states exist or not19. Instead of single DES, according to NB-BBC, two end states are predicted to separately locate at the two opposite sides, or both locate at one (left or right) side.

So, the situation becomes confusing: according to numerical calculations, there exist DESs in NH topological systems. To accurately predict the existence of single DES, one should obtain the topological phase diagram to know whether the edge states exist and check the number of the edge states to know whether the edge states become defective. However, neither the fractional winding number nor the non-Bloch topological invariants accurately predict the existence of single DES. There is a puzzle: how to understand the existence of the DESs?

In this paper, we try to resolve this puzzle after answering the following questions:

1. What’s the underlying physics of the DESs?
2. How to accurately characterize the DESs?
3. Are the DESs stable in thermodynamic limit?
4. Does there exist universal features of DESs?

The key point of the answers is which the number of the edge states becomes anomalous due to the existence of DESs that distinguishes NB-BBC with phase-boundary anomaly. We call the anomalous BBC with the number anomaly of the edge states A-BBC for short.
Quantitative description for anomalous bulk-boundary correspondence: Firstly, we consider the boundary physics for an arbitrary 1D finite NH topological system, of which the Hamiltonian is $\hat{H}_{NH}$ ($\hat{H}_{NH} \neq \hat{H}_{NH}^\dagger$). From the classification of NH topological systems\cite{31,32}, in topological phase, the topological invariant $Z$ may guarantee $C_{finite}$ edge states in 1D. The biorthogonal set for the quantum states of the boundary/edge modes is defined by $|b_k\rangle$ and $|\bar{b}_k\rangle$, i.e., $\hat{H}_{NH}|b_k\rangle = E_k|b_k\rangle$, $\hat{H}_{NH}^\dagger|\bar{b}_k\rangle = (E_k)^*|\bar{b}_k\rangle$, and $\langle b_k|\bar{b}_k\rangle = 1$ ($k = 1,...,C_{finite}$ is state index).\cite{33}. The BBC for finite NH topological systems is denoted by $C_{finite} = 2Z$. A-BBC is the number anomaly of the edge states, i.e., the number of the edge states is not to be $2Z$ even in thermodynamic limit,

$$C_{finite} \neq 2Z. \quad (1)$$

A special case of A-BBC is $C_{finite} = Z$ that indicates the existence of a DES. We emphasize that the DES may have a distribution on both edges.

In this paper, we focus on 1D finite NH topological system with $Z = 1$. To quantitatively characterize the edge physics for a 1D finite NH topological system, we introduce an effective edge Hamiltonian,

$$\hat{H}_{edge} = \begin{pmatrix} h_{11} & h_{12} \\ h_{12} & h_{22} \end{pmatrix} \quad (2)$$

where $h_{IJ} = \langle b^I | \hat{H}_{NH} | b^J \rangle$, $I, J = 1, 2$, $| b^1 \rangle$, $| b^2 \rangle$ are the basis of the edge states. With the help of $\hat{H}_{edge}$, the boundary phase diagram of the NH topological systems can be obtained straightforwardly.

To develop a clear quantitative description for the DESs and the corresponding A-BBC, we introduce three new concepts:

Definition 1 - Abelian/non-Abelian NH condition: A NH Hamiltonian $\hat{H}$ ($\hat{H} \neq (\hat{H})^\dagger$) can be written into $\hat{H} = \hat{H}_a + \hat{H}_b$ where $\hat{H}_b = \frac{1}{2}(\hat{H} + \hat{H}^\dagger)$ and $\hat{H}_a = \frac{1}{2}(\hat{H} - \hat{H}^\dagger)$ are the Hermitian part and anti-Hermitian part, respectively. A Hamiltonian $\hat{H}$ is Abelian NH if $[\hat{H}_b, \hat{H}_a] = 0$; A Hamiltonian $\hat{H}$ is non-Abelian NH if $[\hat{H}_b, \hat{H}_a] \neq 0$.

When $\hat{H}_{edge}$ obeys non-Abelian NH, we call it anomalous, of which the eigenstates $|\psi_+\rangle$ and $|\psi_-\rangle$ coalesce. Consequently, according to $C_{finite} \neq 2Z$, the BBC becomes anomalous.

Definition 2 - State similarity of edge states: The state similarity for two edge states $|\psi_+\rangle$ and $|\psi_-\rangle$ is $|\langle \psi_+ | \psi_- \rangle|$. Here, $|\psi_\pm\rangle$ is satisfied self-normalization condition, i.e., $|\langle \psi_\pm | \psi_\pm \rangle| = 1$.

Definition 3 - BBC ratio: The BBC ratio is defined by $\Upsilon_{BBC} = 1 - |\langle \psi_+ | \psi_- \rangle|/2 = C_{finite} = 2Z$. $\Upsilon_{BBC}$ is the total number of edge states for a finite NH system. $| \psi_\pm \rangle$ are the two edge states. $\Upsilon_{BBC}$ is a quantity that characterizes number anomaly of the edge states.

If $\Upsilon_{BBC}$ is 1, there exists the usual bulk-boundary correspondence; if $\Upsilon_{BBC}$ is smaller than 1, there exists A-BBC. And if $\Upsilon_{BBC}$ is equal to 1/2, there exists DES. The existence of DESs and A-BBC in NH topological systems becomes a well defined mathematical problem under quantitative calculations. The detailed proof of this statement is given in supplementary materials.

The defective edge states as boundary exceptional points in nonreciprocal Su-Schrieffer-Heeger model: We take 1D nonreciprocal Su-Schrieffer-Heeger (SSH) model as an example to explore the underlying physics of A-BBC and DESs. The Bloch Hamiltonian for a nonreciprocal SSH model with $N$ pairs of lattice sites under PBC is given by

$$\hat{H}_{NH-SSH} = (t_1 + t_2 \cos k) \sigma_x + (t_2 \sin k + i\gamma) \sigma_y. \quad (3)$$

t_1 and $t_2$ describe the intra-cell and inter-cell hopping strengths, respectively. $\gamma$ describes the unequal intra-cell hoppings. $k$ is wave-vector. $k$, $t_1$, $t_2$, $\gamma$ are all real. $\sigma_i$’s are the Pauli matrices acting on the (A or B) sublattice subspace. In this paper, we set $t_2 = 1$. For this case, there exists chiral symmetry, $\sigma_z \hat{H}_{NH-SSH}(k) \sigma_z = -\hat{H}_{NH-SSH}(k)$.

Firstly, we consider the Hermitian SSH model with $\gamma = 0$. Now, the topological invariant is a winding number $w = \frac{1}{2\pi} \int_{-\pi}^\pi \partial_k \phi(k) \cdot dk$ where $\phi(k) = \tan^{-1}(d_y/d_x)$ with $d_y = t_2 \sin k$ and $d_x = t_1 + t_2 \cos k$. There are two phases for the global bulk phase diagram, topological phase with $w = 1$ in the region of $|t_1| < |t_2|$ and trivial phase with $w = 0$ in the region of $|t_1| > |t_2|$. In topological phase, the basis of the edge states is given by $| b^1 \rangle, | b^2 \rangle$, of which the wave-function is $| b^1 \rangle = \frac{1}{\sqrt{2}} \sum_{n=1}^N (-\frac{t_2}{t_1})^{n-1} |n\rangle \otimes | 1 \rangle$ or $| b^2 \rangle = \frac{1}{\sqrt{2}} \sum_{n=0}^{N-1} (-\frac{t_2}{t_1})^n |N-n\rangle \otimes | 0 \rangle$ where $N = \sqrt{(1-(\frac{t_2}{t_1})^2)/((1-(\frac{t_2}{t_1})^2)$ is normalization factor, and $| 1 \rangle$ and $| 0 \rangle$ denote the state vectors of two-sublattices. The orthogonal condition for the two edge states is $\langle b^1 | b^2 \rangle = 0$. To characterize the dynamics of the two edge states of finite NH SSH model, we derive the edge Hamiltonian, $\hat{H}_{edge} = \begin{pmatrix} h_{11} & h_{12} \\ h_{12} & h_{22} \end{pmatrix}$ where $h_{11} = \langle b^1 | \hat{H}_{NH-SSH} | b^1 \rangle$, $I, J = 1, 2$. For this case, we have $h_{11} = -h_{22} = 0$, $h_{12} = h_{21} = \Delta_0 = (\frac{t_1+t_2}{t_2})(-\frac{t_1}{t_2})^{N}$ and obtain an effective edge Hamiltonian for Hermitian SSH model

$$\hat{H}_{edge} = \Delta_0 \cdot \tau_x \quad (4)$$

where $\tau_i$’s are the Pauli matrices acting on the subspace of two edge states.

When consider the unequal intra-cell hoppings ($\gamma \neq 0$), the DESs appear. Correspondingly, the NB-BBC becomes anomalous.

Under OBC, to deal with NH skin effect\cite{19,20}, we do a similar transformation, i.e., $\hat{H}_{NH-SSH} = (\Delta_{NHP})^{-1} \hat{H}_{NH-SSH} \Delta_{NHP} = (t_1 + t_2 \cos k)\sigma_x + t_2 \sin k \sigma_y$.
where $\hat{S}_{NHP}$ is the operator for similar transformation. Under $\hat{S}_{NHP}$, we remove the imaginary wave-vector, i.e., $|\psi(k)\rangle \rightarrow |\psi(k)\rangle' = (\hat{S}_{NHP})^{-1} |\psi(k-iq_0)\rangle$ by doing NH transformation $U_{NHP} = \begin{pmatrix} 1 & 0 \\ 0 & e^{-q_0}\end{pmatrix}$ and site-dependent scaling transformation $|n\rangle \rightarrow |n\rangle' = e^{-q_0(n-1)}|n\rangle$ ($n$ denotes the cell number). $q_0$ is the real value of imaginary wave-vector, $e^{q_0} = \sqrt{t_1 - \gamma}/\gamma$. Consequently, the effective hopping parameters become $\bar{t}_1 = \sqrt{(t_1 - \gamma)(t_1 + \gamma)}$, and $\bar{t}_2 = t_2$. Now, the topological transition occurs at $|t_1| = |t_2|$. In the topological phase $|t_1| < |t_2|$, the edge states are protected by the non-Bloch topological invariants determined by $\hat{H}_{NH-SSH}$ [19–20], $w = \frac{1}{2\pi} \int_{\pi} \partial\phi(k)dk$, where $\phi(k) = \tan^{-1}(d_y/d_x)$ and $d_x = \bar{t}_1 + \bar{t}_2 \cos k$, $d_y = \bar{t}_2 \sin k$. Due to $w = 1$, based on biorthogonal set, the basis of the edge states is given by $\{ \bar{b}^1, \bar{b}^2 \}$, of which the wave-function is $|\bar{b}^1\rangle = \frac{1}{N} \sum_{n=1}^{N} (\frac{x}{\bar{t}_2} e^{i\gamma_0 n})^{-1} |n\rangle \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, or $|\bar{b}^2\rangle = \frac{1}{N} \sum_{n=0}^{N-1} (\frac{x}{\bar{t}_2} e^{-i\gamma_0 n}) |N-n\rangle \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ where $N' = N(t_1 \rightarrow \bar{t}_1, t_2 \rightarrow \bar{t}_2) = \sqrt{1 - \left( \frac{t_1 - \gamma}{\bar{t}_2} \right)^2}/(1 - \left( \frac{t_1 - \gamma}{\bar{t}_2} \right)^2)$ is normalization factor. Because the system with $t_1 = \sqrt{(t_1 - \gamma)(t_1 + \gamma)} = 0$ is singularity that corresponds to EPs of all bulk states, in this paper we focus on the case of $t_1 \neq 0$.

Under similar transformation $t_1 \rightarrow \bar{t}_1$, $t_2 \rightarrow \bar{t}_2$, the effective edge Hamiltonian becomes

$$\hat{H}_{edge}(t_1, t_2) = \Delta_0 \cdot \tau^x,$$

where $\Delta = \frac{\sqrt{t_1^2 - t_2^2}}{\bar{t}_2} (\frac{t_1}{\bar{t}_2})^N$. The energy levels are correct that are $E_{\pm} = \pm \Delta$. However, although energy levels are correct, the detailed numerically calculations cannot support this effective edge Hamiltonian $\hat{H}_{edge}$, for example, in numerical results $h_{12} = \langle \bar{b}^1 | \hat{H}_{NH-SSH} | \bar{b}^2 \rangle \neq h_{21} = \langle \bar{b}^2 | \hat{H}_{NH-SSH} | \bar{b}^1 \rangle$. What’s wrong with $\hat{H}_{edge}$? The mismatch comes from overlooking NH polarization effect on the two edge states.

To derive the correct result, we must consider an additional NH boundary polarization operation on edge modes, $\tau^x \rightarrow U_{edge}^{-1} \tau^x U_{edge} = \tau^x \cosh(q_0 N) - i\tau^y \sinh(q_0 N)$ where

$$U_{edge} = \begin{pmatrix} 1 & 0 \\ 0 & e^{-q_0 N} \end{pmatrix}.$$

After considering $U_{edge}$, the effective spin model $\hat{H}_{edge}$ becomes anomalous, i.e.,

$$\hat{H}_{eff} = (U_{edge})^{-1} \hat{H}_{edge}(U_{edge}) = \begin{pmatrix} 0 & \Delta e^{-q_0 N} \\ \Delta e^{q_0 N} & 0 \end{pmatrix} \Delta^x \tau^x - i\Delta^y \tau^y,$$

where $\Delta^x = \Delta \cosh(q_0 N)$, $\Delta^y = \Delta \sinh(q_0 N)$. Under $U_{edge}$, the energy levels doesn’t change, $E_{\pm} = \pm \Delta$. In Fig.1(a), we also numerically calculate the two matrix elements for the case of $N = 15$ and eventually find the consistence between the numerical results and analytical results.

There exists emergent chiral symmetry and effective $\mathcal{PT}$-symmetry for the edge Hamiltonian $\hat{H}_{eff}$ [53–57], i.e.,

$$\tau_z \hat{H}_{eff}(k) \tau_z = -\hat{H}_{eff},$$

and

$$[\mathcal{P}_{eff} \mathcal{T}, \hat{H}_{eff}] = 0, \mathcal{P}_{eff} = \tau^z.$$

This anomalous edge Hamiltonian $\hat{H}_{eff}$ obeys non-Abelian NH condition. The condition for boundary EPs is obtained as $|\Delta| = 0$. The solution for this equation is $N \rightarrow \infty$ or $|t_1| = |\gamma|$. As shown in Fig.1(b), the red region corresponds to boundary EPs. Thus, the two edge states merge into one at boundary EPs $|t_1| = |\gamma|$ or $N \rightarrow \infty$, of which the wave-function is $|\psi_+\rangle = |\psi_-\rangle = |\bar{b}^1\rangle$ or $|\bar{b}^2\rangle$. In thermodynamic limit, the edge state for $E = 0$ becomes defective and is localized either on the left edge or the right edge. Let us discuss the A-BBC in this condition. The figure of $\tau_{BBC}$ in Fig.1(b) is plotted for NH topological system with finite size $N = 10$. In thermodynamic limit $N \rightarrow \infty$, for the case of $t_1 \neq 0$ and $\gamma \neq 0$, the anomalous edge Hamiltonian becomes

$$\hat{H}_{eff} \rightarrow \Delta^x \tau^x, (\tau^x = \tau^x \pm i\tau^y)$$
that also obeys non-Abelian NH condition. Now, we have the state similarity $|\psi_+\rangle = \tanh(2q_0N)$ to be 1 and the BBC ratio $\Upsilon_{BBC}$ turns to $1/2$. In particular, as shown in Fig.1(d), the BBC for the NH topological system in thermodynamic limit $(t_1 \neq 0 \text{ and } \gamma \neq 0)$ is anomalous! For the case of $t_1 = 0$ and $\gamma = 0$, the edge Hamiltonian $\hat{H}_\text{eff}$ becomes usual and the corresponding $\Upsilon_{BBC}$ turns to 1.

Stability of defective edge states in thermodynamic limit: To examine the stability of the DESs, we add an additional imaginary staggered potential $i\varepsilon z$ on $H_\text{NH-SSH}$. Using a similar approach, the anomalous edge Hamiltonian is obtained as

$$\hat{H}_\text{eff} = \bar{\Delta}_x \tau_x - i\bar{\Delta}_y \tau_y + i\varepsilon \tau^z$$  \hspace{1cm} (11)

where $\bar{\Delta} = \bar{\Delta}_x = \bar{\Delta}_y = \bar{\Delta}_z = \bar{\Delta}_y = e^{\varepsilon_0} = \sqrt{\frac{t_1 + t_2 + t_3 + t_4}{1, t_2}} (\frac{t_1^2 - t_2^2 - t_3^2}{t_2} - \varepsilon_x)^{N/2}$. A spontaneous (effective) $\mathcal{PT}$ symmetry-breaking transition occurs at the boundary EPs $|\bar{\Delta}| = |\varepsilon|$. For a finite system, the DES for boundary EPs described by $|\psi_+\rangle = |\psi_-\rangle = \frac{1}{\sqrt{1 + i e^\varepsilon N}} (|b_1\rangle - i e^{\varepsilon N} |b_2\rangle)$. This is DES without chiral symmetry that is no more localized either on the left edge or on the right edge.

In thermodynamic limit, according to $\bar{\Delta} \to 0$, for the case of $\varepsilon \neq 0$, the edge Hamiltonian obeys Abelian NH condition $\hat{H}_\text{edge} \to i\varepsilon \tau^z$. The BBC ratio $\Upsilon_{BBC}$ turns into 1 and the BBC becomes usual. That means, in thermodynamic limit, arbitrary imaginary staggered potential breaking chiral symmetry changes the effect from NH boundary polarization ($|\varepsilon| \gg |\bar{\Delta}| \sim (\frac{t_1^2 - t_2^2}{t_3} - \varepsilon_x)^{N/2} \to 0$) and moves the edge Hamiltonian away from boundary EPs. As a result, in thermodynamic limit, for a general NH SSH model without the protection of chiral symmetry, the DES is unstable.

A-BBC theorem for number anomaly of the edge states in a general non-Hermitian topological system: To develop general formula, we consider an arbitrary 1D NH topological system with topological invariant $Z$, of which the Hamiltonian is $H_\text{NH}$. To explore the universal features for A-BBC from DESs, we prove the following A-BBC theorem.

A-BBC theorem: The usual BBC is satisfied if the boundary/edge Hamiltonian $\hat{H}_\text{edge}$ ($\hat{H}_\text{edge} \neq (\hat{H}_\text{edge})^\dagger$) for a NH topological system obeys Abelian NH condition, $[\hat{H}_\text{edge}, \hat{H}_\text{edge,a}] = 0$. Now, $\Upsilon_{BBC}$ is 1; On the contrary, the BBC becomes anomalous if the $\hat{H}_\text{edge}$ obeys the non-Abelian NH condition, $[\hat{H}_\text{edge}, \hat{H}_\text{edge,a}] \neq 0$. Now, $\Upsilon_{BBC}$ is smaller than 1. Here, $\hat{H}_\text{edge} = \frac{1}{2}(\hat{H}_\text{edge} + (\hat{H}_\text{edge})^\dagger)$ and $\hat{H}_\text{edge,a} = \frac{1}{2}(\hat{H}_\text{edge} - (\hat{H}_\text{edge})^\dagger)$. In supplementary materials, we show the detailed proof of BBC theorem.

A special case of A-BBC is $\Upsilon_{BBC} = 1/2$ that corresponds to boundary EPs with the DES. Now, the anomalous edge Hamiltonian $\hat{H}_\text{edge}$ ($\hat{H}_\text{edge} \neq (\hat{H}_\text{edge})^\dagger$) obeys the following conditions, $\{\hat{H}_\text{edge}, \hat{H}_\text{edge,a}\} = 0$ and $\hat{H}_\text{edge,h} = T(\hat{T} \cdot \hat{H}_\text{edge,a})T^{-1}$ (here, $T$ is an unitary Hermitian matrix).

Conclusion and discussion: In the end, we draw a brief conclusion. In this paper, the puzzle "how to understand the existence of the DESs" is resolved. The theory of A-BBC for DESs is developed that distinguishes the NB-BBC from NH skin effect. A rigorous theorem – A-BBC theorem is proved. With the help of this theorem, the A-BBC of number anomaly of the edge states is identified by verifying the NH condition of effective edge Hamiltonian $\hat{H}_\text{edge}$. A special case of $\Upsilon_{BBC} = 1/2$ corresponds to boundary EPs and there exists a DES with $E = 0$. For the NH SSH model with chiral symmetry, unequal intra-cell hoppings cause NH boundary polarization that drives the edge states to boundary EPs. That means that there is no intrinsic relationship between the DES with zero energy and the fractional winding number for the bulk state under PBC\cite{11,22}. The NB-BBC from NH skin effect for bulk states is relevant to the correct topological phase diagram but not the defective zero edge modes (nor the number anomaly of the edge states)\cite{13,20}. In addition, we emphasize that the quantitative theory for A-BBC of number anomaly of the edge states can be generalized to various types of NH topological systems, for example, 1D NH SSH model with next-next nearest neighbour hoppings, 1D NH topological superconductors and two dimensional NH topological insulators. These issues will be presented in future.

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