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Why does bulk boundary correspondence fail in some non-hermitian topological models

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Abstract

The bulk-boundary correspondence is crucial to topological insulators. It associates the existence of boundary states (with zero energy and possessing chiral or helical properties) with the topological numbers defined in bulk. In recent years, topology has been extended to non-hermitian systems, opening a new research area called non-hermitian topological insulator. In this paper, however, we will illustrate that the bulk-boundary correspondence does not hold in these new models. This is because a prerequisite condition: 'the boundaries cannot alter most of the bulk states, so as to the topological numbers defined on them' does not hold any longer. This cuts out the correspondence between the topological numbers and the boundary states. We will illustrate that, as approaching the open boundary condition by eliminating the strength of the hopping between the two ends of a chain, a new series of exceptional points must be passed through and the topological structure of the spectrum in the complex plane has been changed. This makes the spectrum topology different for the chains with and without boundaries. We also discuss that such exotic behavior does not emerge when the open boundary is replaced by a domain-wall. So the index theorem can be applied to the systems with domain-walls but cannot be further used to those with open boundaries.

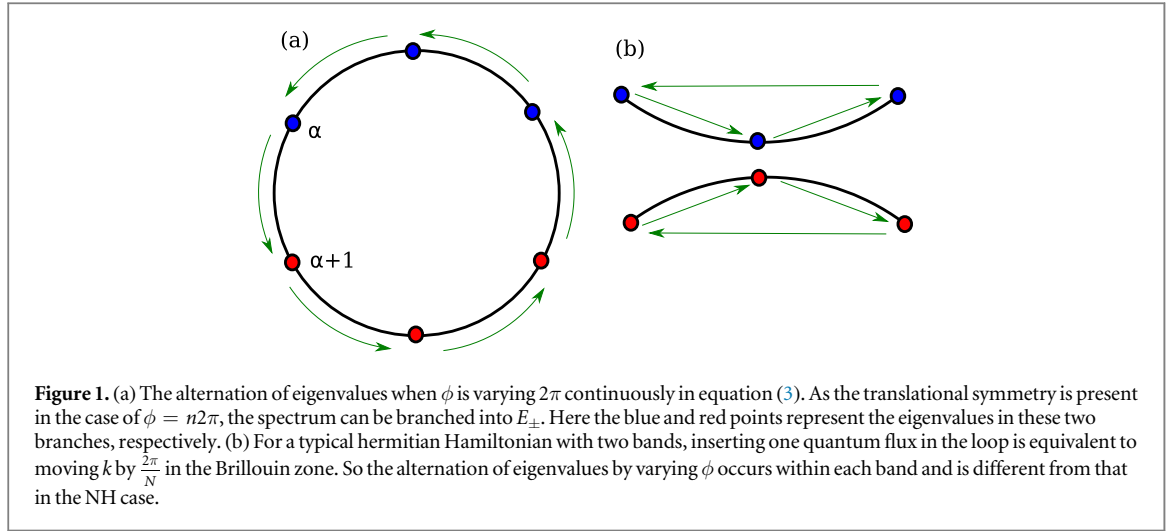
1. Introduction

In quantum mechanics with hermitian Hamiltonian, the degeneracy of the energy levels is the source of the topological order, e.g., the nonzero (first kind of) Chern number is generated by the effective magnetic monopoles at the degenerate points in a parameter space [1]. In the last decade, some authors try to spread these ideas to the models with non-hermitian (NH) Hamiltonian [2–8]. Besides the topological phase that is smoothly extended from the hermitian cases [5, 9], the NH models can possess new topological phases stemming from a new kind of degenerate points, the *exceptional points* (EPs) [10–18].

The discussions on the NH Hamiltonian started more than half a century ago and a special kind of NH models, \mathcal{PT} -symmetric models, has been studied both theoretically and experimentally [13–15, 19–52]. EPs are the special points in a parameter space where the NH matrix ceases to be diagonalizable because of the coalescences of the eigenvalues and eigenstates. These properties can be illustrated by the following 2×2 Jordan block reading as

$$H = \begin{pmatrix} 0 & 1 \\ r_0 e^{-ik} & 0 \end{pmatrix}. \quad (1)$$

The EP at $r_0 = 0$ is the point where the two eigenvalues coalesce to 0 and the right eigenstates (left eigenstates) coalesce to $(1, 0)^T$ ($(0, 1)$). As there is only one eigenstate, the Jordan block cannot be diagonalized any more at the EP. An EP can induce a square root singularity so that there are multiple square root branches in the parameter space around it. It can be illustrated by encircling the EP by varying k from 0 to 2π in the above matrix. The two eigenvalues read



$$E_{\pm} = \sqrt{r_0} e^{ik}. \quad (2)$$

Due to the two branches in the complex plane induced by the square root, the eigenvalues that continuously varying with k will come back to their original values after 4π instead of a 2π period for the matrix itself. This fact leads to the studies of NH topological insulators [7, 8].

In the previous comment [53], we question whether it is necessary to connect the square root branches with fractional winding number in a topological language [7, 8]. In this article, we further prove that there is no bulk-boundary correspondence in several NH models. In these models, the zero energy boundary states (ZEBs) are created by the open boundary condition that is just at an EP of the Hamiltonian (as the open boundary condition is at the EP $r = 0$ of Hamiltonian (3)), or is exponentially close to an EP (as the open boundary condition at $r = 0$ which is exponentially close to an EP at $r_c \sim e^{-\alpha N}$ of Hamiltonian (7)). This is different from the ZEBs that are protected by the chiral symmetry in the traditional hermitian topological insulators. As the open boundary is accompanying with EP while a domain-wall does not, the index theorem presented in [8] can only be applied to the systems with domain-wall but cannot be further extended to the systems with open boundary condition (OBC). Besides that, many exotic properties emerge, i.e., *all* bulk states are changed from extended states to the exponentially localized states only by a change of the boundary condition from periodic to open.

2. Models and results

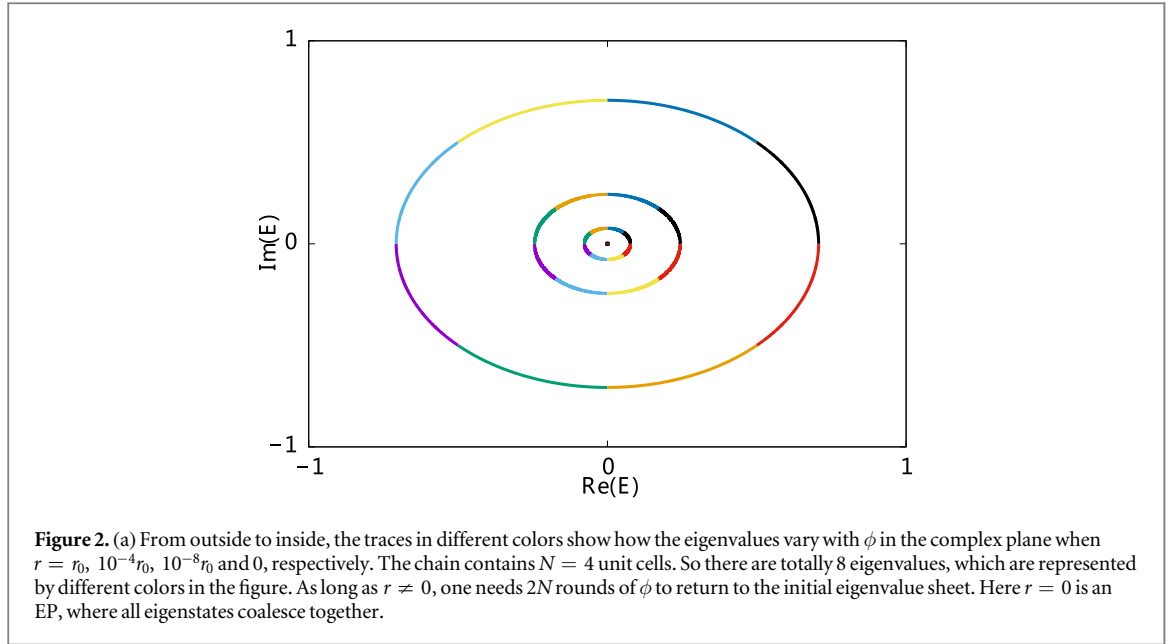
We start this section with the toy matrix in equation (1) because it will illustrate many exotic features associated with EP. We will talk about two kinds of EPs. When the Hamiltonian is presented in the momentum space, the first kind of EP, ($r_0 = 0, k = \text{any}$), is in a polar coordinated space spanned by the parameter r_0 (radius) and the wave-vector k (azimuth).

After a Fourier transformation, the parameter r_0 is representing the strength of hoppings between the nearest neighboring unit cells and the unity on the up-right corner of the matrix in equation (1) specifies the intra-unit-cell hoppings. Here we will use the letters A and B to denote the inequivalent atoms in each unit cell. In this real space representation, there is a particular hopping term between the two ends of the chain whose strength and phase are denoted by the new parameters, r and ϕ , respectively. Obviously, we can approach the open boundary condition by taking $r = 0$. ϕ , here, is used to connect with the wave-vector k in equation (1). When $r = r_0$, one can understand this by a gauge transformation that transforms all the related phases e^{ik} between the nearest neighboring unit cells to a phase jump $e^{i\phi} = e^{iNk}$ across the two ends. Here N is the length of the chain (the number of the unit cells). Such connection between ϕ and k has been employed more than three decades [54] and it is easy to verify that varying ϕ by 2π is equivalent to a shift of $\frac{2\pi}{N}$ for k in the Brillouin zone, as will be shown in figures 1 and 2. The second kind of EPs we will discuss is in the parameter space spanned by r (radius) and ϕ (azimuth).

We can explicitly write down the above Hamiltonian in the real space,

$$H = \sum_{l=1}^N c_{l,A}^{\dagger} c_{l,B} + \sum_{l=1}^{N-1} r_0 c_{l,B}^{\dagger} c_{l+1,A} + r e^{i\phi} c_{N,B}^{\dagger} c_{1,A}. \quad (3)$$

Without loss of generality, we take r_0 to be real and positive. The last term represents the hopping between the two ends. When $r = r_0$ and $\phi = 0$, the translational symmetry restores and the spectrum can be grouped into two branches by $E_{\pm}(k) = \pm \sqrt{r_0} e^{ik/2}$ with N discrete k . In figure 1(a), we schematically show the eigenvalues on a



circle in the complex plane and the colors are used to distinguish the two branches. For the sake of clarity in our next discussion, we relabel these eigenvalues along the circle counterclockwise by E_α , where $\alpha = 1, 2, \dots, 2N$. Then we adjust ϕ from 0 to 2π continuously in equation (3). The $2n$ th-root of the complex number implies that E_α is continuously changed to $E_{\alpha+1}$ and E_{2N} is changed to E_1 . We want to emphasize that this pumping property is distinct from that in the hermitian case and our general discussions will be based on it. In figure 1, we schematically show this distinction.

Next, we consider the effect of boundary by decreasing r . In figure 2, we show how the eigenvalues evolve with ϕ in a $N = 4$ chain when $r = X^{2N}r_0$. In the figure, X^{2N} is taken as 1, 10^{-4} , 10^{-8} and 0, respectively. Actually, When $r \neq r_0$, equation (3) can still be mapped back to a translational symmetric matrix by a non-unitary transformation,

$$H \rightarrow V^{-1}HV, \quad (4)$$

with $V = \text{diag}(1, X, X^2, \dots, X^{2N-1})$. Here V is a matrix with only diagonal elements 1, X, \dots, X^{2N-1} . After the transformation, the difference between the hopping amplitudes at the boundary and in the bulk is smeared out and the hoppings in bulk are rescaled by X . This is why only the radius but not the shape of the circle is changed as r is decreasing. We also notice that the above transformation indicates that all the right eigenstates becomes exponentially localized on the left end of the chain while the left eigenstates localizes on the right end, which are confirmed by the numerical calculations.

Here $r = 0$ is an EP of the Hamiltonian in equation (3). Actually, this is a $2N$ degenerate EP with $2N$ eigenvalues coalescing to $E = 0$. All the right and the left eigenstates coalesce to $(1, 0, \dots)^T$ and $(0, \dots, 1)$, respectively. And we need to encircle this EP (by taking $r \neq 0$ and $\phi = 0 \rightarrow 2\pi$) $2N$ rounds to reach the initial sheet of the eigenstates. One should note that in the momentum space, the toy model is encircling an EP as varying k without touching any EP. But in the real space representation, when the OBC is taken, the model is right at an EP and the Hamiltonian matrix becomes defective. As the spectrum and the eigenstates are changed entirely in approaching OBC, we have to understand the ZEBs from the coalescence of eigenstates at the EP instead of the topological protection of boundary states caused by the bulk (fractional) winding numbers. One reason is that the bulk spectrum has been dramatically changed when the OBC is approached. This makes it impossible to connect the topological band structure in the momentum space to the boundary states in the real space because the two bulk spectra with and without OBC are totally different. So the index theorems, such as the Thouless pump [55], cannot be applied any more. We will present the other reasons after the studies of several models.

In the momentum space, the 1D model in [7] is

$$H_k = (v + r_0 \cos(k))\sigma_x + (r_0 \sin(k) + i\gamma/2)\sigma_z. \quad (5)$$

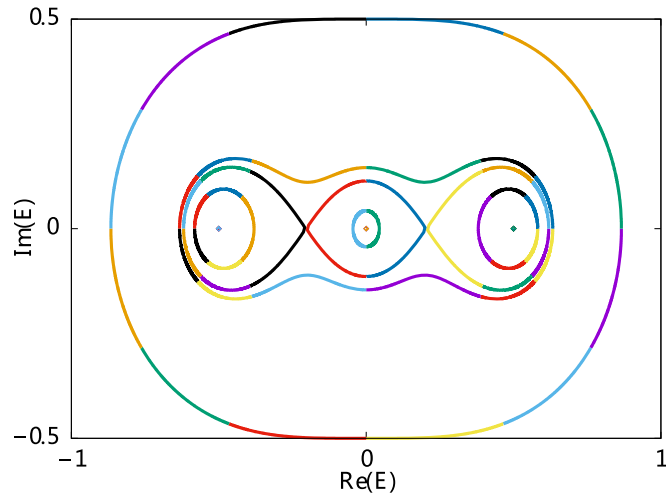


Figure 3. (a) The traces in different colors show how the eigenvalues are evolving when $\phi = 0 \rightarrow 2\pi$. From outside to inside, r is taking 0.5 , 1×10^{-3} , 5.23×10^{-4} , 6×10^{-5} and 0 , respectively. When $r = r_c = 5.23 \times 10^{-4}$, the Hamiltonian encounters an EP at which two pairs of eigenvalues coalesce. As further decreasing r , the alternation of eigenvalues splits into three unconnected loops. When $r = 0$, there is another EP at which the eigenvalues coalesce to three points, 0 and ± 0.5 . Here the length of the chain is $N = 6$. Enlarging the chain does not change the evolution qualitatively, but r_c will exponentially decrease to 0 .

After a unitary transformation $U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}$, $H_k \rightarrow U^\dagger H_k U$, the Hamiltonian changes to

$$H_k = i \begin{pmatrix} 0 & (\gamma/2 - \nu) - r_0 e^{ik} \\ (\gamma/2 + \nu) + r_0 e^{-ik} & 0 \end{pmatrix}. \quad (6)$$

The EPs are at the points where either of the off-diagonal elements is zero. We first take $\gamma = 1$, $\nu = -0.5$ and $r_0 = 0.5$, which are in the topological phase with fractional winding number in [7]. Similar to the toy model in the above discussion, we write down the Hamiltonian in the real space as

$$H = i \left\{ \sum_{l=1}^N c_{l,A}^\dagger c_{l,B} + \sum_{l=1}^{N-1} 1/2 [c_{l,B}^\dagger c_{l+1,A} - c_{l+1,A}^\dagger c_{l,B}] \right. \\ \left. + r [e^{i\phi} c_{N,B}^\dagger c_{1,A} - e^{-i\phi} c_{1,A}^\dagger c_{N,B}] \right\}, \quad (7)$$

where r and ϕ are the amplitude and the phase of the hopping between the two ends of the chain, respectively.

In figure 3, we show how the energy spectrum is varying with ϕ in a $N = 6$ chain for several values of r . When r is relatively large, it still needs totally $2N$ rounds to restore the initial sheet of the eigenvalues because each round shifts the adjacent energy levels one by one counterclockwise. When r is smaller than a critical value, $r < r'_c$, the circular alternation splits into three parts, in which each of two sideward ones contains $N - 1$ states and the middle one has two states. So one will need $2(N - 1)$ rounds to reach the initial spectrum sheet when N is an even number or $(N - 1)$ rounds when N is odd. When r is further decreased to 0 , which corresponds to the chain with OBC, the three circles shrink to three points at ± 0.5 and 0 , respectively. So $r = 0$ is also an EP of the Hamiltonian in the real space. But the degeneracy of this EP is smaller than that in the above toy model. Actually, there are totally three EPs at $r = 0$, whose degeneracies are $N - 1$, 2 and $N - 1$, respectively. One should remember that there is also another EP at $(r = r'_c, \phi = \pi)$, where two pairs of eigenvalues coalesce.

We also calculate the evolution of the spectrum for longer chains. The circular alternations are similar to those in the short chain presented in the above figure but the EP at $r = r'_c$ is exponentially rapidly moved to the EP at the origin as the length of the chain is increased.

We plot the results when the parameters are changed to $\gamma = 1$, $\nu = -0.6$ and $r_0 = 0.5$ in figure 4(a). In this case, the center EPs at $r = 0$ is split into many EPs and are moved away from the origin. As figure 4(a) shows, when r is decreased to 0.001 , one EP has been encountered and the traces of eigenvalues are split into three parts with a center large loop containing 10 eigenvalues and the two satellite circles each containing 1 eigenvalue. As further decreasing r , more EPs are encountered and more and more eigenvalues are segregated from the center circle. When $r = r_c = 3 \times 10^{-5}$, the last two eigenvalues at the center coalesce. As all eigenvalues evolve to themselves when $r < r_c$, there is no EP anymore. So in this model, $r = 0$ is not an EP and there are only two bound states near the zero energy when the OBC is finally reached. But when the length of the chain is increased to $N = 20$, whose results have been shown in figure 4(b), all EPs shrink toward 0 rapidly. The last two adherent eigenvalues coalesce at a much smaller $r_c \sim 5.3 \times 10^{-15}$ and stay more close to the zero energy when $r = 0$. So

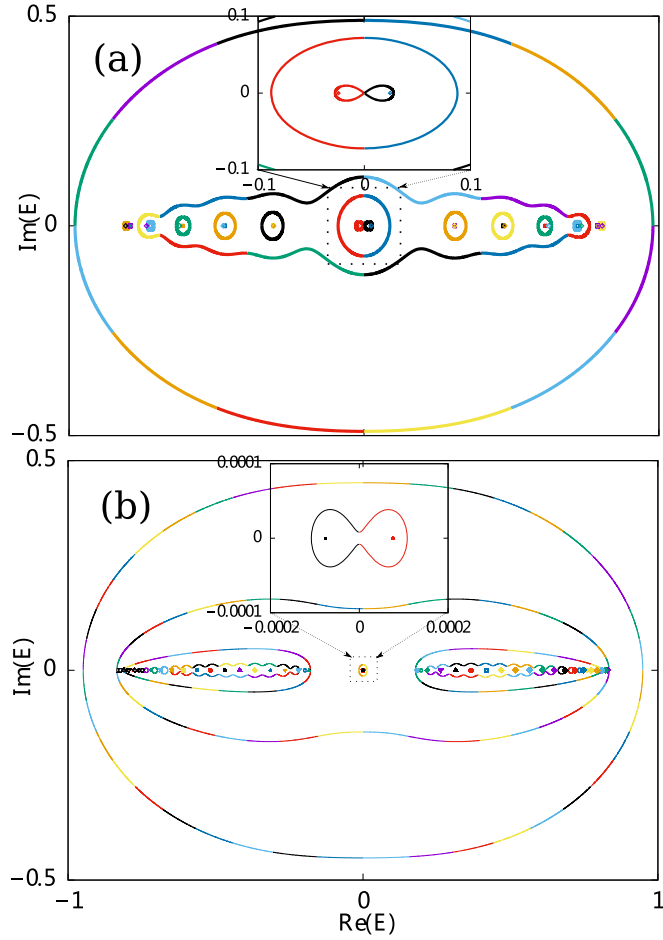


Figure 4. (a) The traces of the eigenvalues when the parameters are changed to $\gamma = 1$, $\nu = -0.6$ and $r_0 = 0.5$ in equation (7). Here from outside to inside, r is taking 0.5 , 1×10^{-3} , 5×10^{-4} , 3.2×10^{-5} and 0 , respectively. A zoom of the original region is shown in the inset. The length of the chain is still $N = 6$. (b) The traces of the eigenvalues when the length of the chain is changed to $N = 20$. Here r is taking 0.5 , 1×10^{-6} , 1×10^{-9} , 1×10^{-10} , 5.3×10^{-15} and 0 , respectively. The inset shows the mini circle and the saturate points when $r = 5.3 \times 10^{-15}$ and 0 .

we can conclude that even $r = 0$ is not an EP in this case, all EPs are moving toward it exponentially rapidly with enlarging the system.

The 2-dimensional(2D) model in [8] reads as

$$H_k = B_x(k_x, k_y)\sigma_z + B_y(k_x, k_y)\sigma_x, \quad (8)$$

where k_x and k_y are the wave-vectors in the x and y directions, respectively. Although this is a 2D model, the authors had considered k_y as a parameter and characterize the topological property by the fractional winding number in the k_x direction. So this model will be equivalent to the previous model in equation (6).

3. Discussions

In real space representation, when the translational symmetry is restored by taking the amplitude of the hopping between the ends equal to that in bulk, $r = r_0$, the variation of ϕ by 2π is equivalent to the shift of the wave-vector k by $\frac{2\pi}{N}$ in the Brillouin zone. As the period of the energy spectrum with k is 4π in the momentum space, their period with ϕ in the real space must be $4N\pi$ instead of $2N\pi$. On the complex plane ($r \cos(\phi)$, $r \sin(\phi)$), there must be several EPs inside the circle $|re^{i\phi}| = r_0$ because when $r = 0$ all eigenvalues must not varying with ϕ any longer. For equation (7) with $\gamma = 1$, $\nu = -0.5$ and $r_0 = 0.5$, after writing down the Hamiltonian matrix with OBC, $r = 0$, one can immediately realize that this is an EP and there are at least two eigenvalues coalesce to zero energy. We suggest to attribute this ZEBS to the EP instead to the topological protected boundary state for the following reasons.

Firstly, as we mentioned previously, the spectrum of the models with OBC or with periodic boundary condition are sharply different. All the states, including the ZEBS, are exponentially localized at the boundary in

the former case, but are extended in the latter case. This distinction makes the two systems uncorrelated so that the topological numbers defined in the latter system has nothing to do with the spectrum when the OBC is taken.

Secondly, the fractional winding number defined in the momentum space is stemmed from the 4π period of k . In real space, it has been inherited by the $4N\pi$ period of ϕ when $r = r_0$. So we can conclude that the topological number (fractional winding number here) is encoded in the topology of the traces of the eigenvalues. To reach OBC as decreasing r , one must encounter EPs and the topology of the traces must be changed (as one large loop splits into smaller loops shown in the previous figures). So it is impossible to associate the ZEBS at the open boundary to the fractional winding number defined without boundary because the topologies of the two systems are entirely different.

Thirdly, the ZEBSs are not protected by the chiral symmetry. They are actually caused by the fact that the Hamiltonian matrix with OBC has two eigenvalues coalesce to zero energy or near the zero energy. We take equation (6) with the parameters $\gamma = 1$, $\nu = -0.5$ and $r_0 = 0.5$ as an example. The definition of the winding number in the momentum space requires a chiral symmetry, which is $\sigma_z H_k \sigma_z = -H_k$ in this article. If the topological understanding of ZEBS is right, they must disappear when a term $h\sigma_z$ is added in the Hamiltonian to break the symmetry. In the real space representation, we recover the EP at $r = 0$ by eliminating the term $h(c_{1A}^\dagger c_{1A} - c_{NB}^\dagger c_{NB})$ in the two unit cells at the boundaries. A simple numerical calculation confirms that the ZEBSs are still present. So even when there is no chiral symmetry and the fractional winding number is undefined, as long as the EP at $r = 0$ is present, the ZEBSs can still exist.

This article questions the topological understanding of ZEBS in NH models. But we are not challenging most of the results in [8] because the authors discussed domain-walls instead of open boundaries there. Unlike the models with open boundaries, a system with domain-walls will not encounter the EP problem. But we want to emphasize that their conclusions on the domain-walls cannot be further extended to the open boundaries. For instance, the index theorem in that article starts from a translation $H' = H^\dagger H$ that maps the NH Hamiltonian H to an hermitian Hamiltonian H' . When H is not defective, the above translation maps the spectrum ϵ to $|\epsilon|^2$ one by one. But the Hamiltonian H will be defective right at the EP so that the spectrum of H' are not mapped one by one to that of H any more. The toy model in equation (1) can illustrate this: the eigenvalues of $H^\dagger H$ are not fixed at zero when $r_0 = 0$. So the index theorem cannot be applied to the chain with OBC.

In the Hermitian models, the topological boundary states bounded on the boundary can be traced back to the mismatch of the Wanniers centers in the modern theorem of the polarization [56]. These Wanniers centers are determined by the whole occupied band of the bulk. This is the physics behind the bulk-boundary correspondence. However, as we just concluded, in the non-hermitian models, the bulk states are inevitably changed by the EPs as approaching the open boundary condition. This is why the correspondence between the bulk band structure and the boundary states is cut off in the open boundary condition of the NH Hamiltonian. If the open boundary condition is replaced with a domain wall, the situation will become different. A domain wall is a boundary that separates two regions with different parameters (such as the media with inverse sign of mass or gap discussed in [8]). The similar polarization argument is still applicable because the domain-wall will not enroll extra EP like open boundary. Thus, as discussed in [8], the bulk-boundary correspondence is applicable provided that the suitable bulk topological numbers are chosen. In [8], two winding numbers obtained from the bulk states are chosen to describe the bulk-boundary correspondence, one is a generalization of the Berry phase to the NH system, another is calculated from the argument of the eigenvalues.

At the end of this section, we want to clarify how will the topology of the spectrum(eigenvalues) relate to the traditional topological winding number defined for the eigenvectors. As we have discussed, ϕ is playing a similar role as the wave-vector k . The nontrivial topological proprieties for the eigenvectors stem from the multiple branches of the eigenvalues which have been inherited by ϕ showing in figure 2. Any topological change of the spectrum from a circle must indicate a change in the topological property of the eigenvectors.

4. Conclusions

We indicate that, as eliminating the amplitude of hopping between the ends of a chain to reach OBC, extra EP must be passed through and the topological structure of the band has been changed. This makes it impossible to associate the ZEBS in the OBC case to the fractional winding number defined without taking into account the boundary effect. The topological index theorem on a domain-wall cannot be naturally extended to that on the boundary for the same reason. The spectrum of the chain with OBC should be studied individually and the topological bulk boundary correspondence is cut out. Our studies also show that there are EPs at or exponentially adjacent to $r = 0$ in a long chain in these models. This makes it possible to study the effect of EP on a long chain without finely tune the parameters.

Technical note: All data shown in this article are calculated by the standard lapack function: zgeev. But near or at the EP, the LU decomposition used by zgeev is unstable when the dimension of the matrix is large. So if one

want to calculate the spectrum for a longer chain, we suggest to use a bi-orthogonal Gram-Schmidt process whose validity has been verified by us.

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