Topological characterization of non-Hermitian multiband systems using Majorana’s Stellar Representation

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For topological characterization of non-Hermitian multiband systems, Majorana’s stellar representation (MSR) is applied to 1D multiband models consisting of asymmetric nearest-neighbor hopping and imaginary on-site potentials. The number of edge states isolated from the continuous bulk bands in the complex energy plane is successfully linked with a topological invariant constructed from MSR. Specifically, the number of isolated edge states can be obtained from a winding number defined for the Majorana stars, which also allows for a geometric visualization of the topology related to the isolated edge modes. A remarkable success of our approach is that our winding number characterization remains valid even in the presence of exceptional points of the continuous bulk bands, where the Hamiltonian becomes non-diagonalizable and hence conventional topological invariants such as the Zak phase and the Chern number cannot be properly defined. Furthermore, cases with the so-called non-Hermitian skin effect are also studied, showing that the bulk-boundary correspondence between our defined winding numbers and isolated edge states can be restored. Of particular interest is a four-band example with an odd number of isolated edge states, where the Zak phase approach necessarily fails upon removing the skin effect, but our MSR-based characterization works equally well. For these reasons, our study is expected to be widely useful in topological studies of non-Hermitian multiband systems, regardless of the skin effect or the presence of the exceptional points in non-Hermitian systems.

I. INTRODUCTION

Non-Hermitian Hamiltonians are now widely recognized to be physically relevant as effective Hamiltonians in many physical systems, such as open quantum systems with finite life time introduced by electron-electron or electron-phonon interactions, and photonic systems with gain and loss. In particular, non-Hermitian topological phases have been one of the most intriguing research subjects during the past few years, because they possess many exotic topological phenomena beyond Hermitian systems. In non-Hermitian systems, exceptional degeneracies emerge when two or more energy levels coalesce into one, becoming identical not only in eigenenergies, but also eigenstates. Such degeneracies can form various manifolds with distinct topological structures in the Brillouin zone of systems beyond one-dimension. The celebrated ten-fold symmetry classification has also been extended into non-Hermitian systems, and is much enriched due to the extra non-spatial symmetries of non-Hermitian matrices. It has also been shown that the non-Hermitian skin effect (NHSE) reflected by enormous accumulation of eigenmodes at system boundaries, can modify the topological bulk-boundary correspondence, and lead to other novel phenomena when interplayed with different physical effects, e.g. non-Hermitian quasicrystal, hybrid skin-
tems and several intriguing examples of multiband systems, we find a one-to-one correspondence between the number of edge states isolated from continuous bands and a winding number defined from these MSs. Remarkably, the winding number we propose is well-defined even when different energy bands coalesce at one or more exceptional points (EPs), whereas conventional topological invariants such as the Zak phase and the Chern number are generally ill-defined in such cases. Furthermore, our method can be directly extended to systems with NHSE via a known procedure, namely, by considering the so-called non-Bloch Hamiltonian obtained by a complex deformation of the quasi-momentum of the studied system. Of particular importance, in a 4-band model with NHSE possessing an odd number of isolated edge states, the Zak phase necessarily fails in this situation. Putting all these results together, it can equally predict the number of edge states in this subtle case, whereas the Zak phase necessarily fails in this situation. Putting all these results together, it can be concluded that our defined winding number provides the most potent topological invariant to date in characterizing non-Hermitian topological phases in multiband systems, where both continuous bands and isolated edge states behave very differently from Hermitian systems.

The rest of this paper is organized as follows. In Sec. II we introduce our multiband models with non-Hermiticity induced by non-reciprocal hoppings and imaginary on-site potentials. In Sec. III we briefly review the MSR of high-(pseudo)spin states, and define a winding number for the MSs of each band. Sec. IV contains the main results of this work, where we illustrate the bulk-boundary correspondence between isolated edge states and our defined winding numbers in several different scenarios with/without EPs and/or NHSE. A brief summary and discussion are given in Sec. V.

II. NON-HERMITIAN 1D MULTIBAND CHAIN MODEL

We consider a 1D lattice model with $J$ lattice sites in a unit cell, as illustrated in Fig. 1. The corresponding tight-binding Hamiltonian is given by

$$H = \sum_n \sum_j (i\mu_j \hat{c}^\dagger_{j,n} \hat{c}_{j,n} + (t_j + \delta_j) \hat{c}^\dagger_{j,n} \hat{c}_{j+1,n} + (t_j - \delta_j) \hat{c}^\dagger_{j+1,n} \hat{c}_{j,n}),$$

(1)

where $\hat{c}_{j,n}$ ($\hat{c}^\dagger_{j,n}$) is the annihilation (creation) operator of a particle at the $j$th lattice site in the $n$th unit cell, and $\hat{c}_{j+1,n} \equiv \hat{c}_{1,n+1}$. Fig. 1 presents a more specific configuration of the lattice. As indicated in Fig. 1 our model consists of $(N \times J)$ lattice sites, with non-reciprocal hopping $t_j \pm \delta_j$ (which may induce NHSE in this system), and on-site imaginary potential $\mu_j$ depicting particle gain and loss.

![FIG. 1: A simple illustration of the non-Hermitian 1D $J$-band chain model. Circles indicate the lattice site and arrows indicate the hopping between the lattices.](image)

By performing the Fourier transformation, $\hat{c}_{j,n} = 1/\sqrt{N} \sum_k e^{imk} \hat{c}_{j,k}$ with $j \in \{1, 2, \ldots, J\}$ to the real space Hamiltonian (1), we can obtain the Bloch Hamiltonian $H_k = \sum_k \psi^\dagger_k h(k) \psi_k$ with $k \in [0, 2\pi]$ being the quasimomentum variable, $\psi_k = \{\hat{c}_{1,k}, \hat{c}_{2,k}, \ldots, \hat{c}_{J,k}\}^T$ and

$$h(k) = \begin{bmatrix}
i\mu_1 & t_1 + \delta_1 & \ldots & 0 & (t_J - \delta_J) e^{-ik} \\
t_1 - \delta_1 & i\mu_2 & \ldots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \ldots & i\mu_{J-1} & t_{J-1} + \delta_{J-1} \\
(t_J + \delta_J) e^{ik} & 0 & \ldots & t_{J-1} - \delta_{J-1} & i\mu_J \
\end{bmatrix}.$$  

(2)

Conventionally, topological properties of 1D Hermitian systems can be characterized by the Zak phase, which is the Berry phase associated with each band as the quasi-momentum $k$ adiabatically runs over one cycle in the Brillouin zone. In particular, when the system consists of only two bands, the Zak phase can be obtained from the solid angle on a Bloch sphere of an eigenstate varying throughout the Brillouin zone, thus providing an intuitive geometric picture of the topology of 1D systems. In non-Hermitian systems, a pair of left and right eigenstates satisfy the biorthogonal normalization condition and the non-Hermitian (always real) Zak phase can be defined as

$$\gamma^{(m)} = -\text{Im} \oint_{BZ} \langle \psi_{L,m}(k) | \partial_k | \psi_{R,m}(k) \rangle dk,$$

(3)

with $\psi_{L,m}(k)$ ($\psi_{R,m}(k)$) the left (right) Bloch eigenstate and $m$ denoting the band index. In a discrete lattice system, by considering discrete wavenumber of $k_n = 2\pi n/N_k$
and \( N_k = N \) as a large integer, the Zak phase can be obtained numerically with
\[
\gamma^{(m)} = -\text{Im} \sum_{n=1}^{N_k} \log[(\psi_{L,m}(k_n)\psi_{R,m}(k_{n+1})].
\]

However, even for a two-band non-Hermitian system, this Zak phase cannot be directly mapped onto a Bloch sphere for visualization, because the definition of left and right eigenstates leads to complex winding angles of the pseudospin vector (see Appendix A). Furthermore, as we illustrate in later discussions, non-Hermitian band structures can host topological edge states even in the presence of exceptional points. In this scenario, the Hamiltonian is not diagonalizable and the Zak phase becomes ill-defined. For these two reasons, a more versatile topological invariant is required to topologically characterize non-Hermitian multiband systems.

### III. THE WINDING NUMBER OF THE MAJORANA STARS

MSR is conventionally used to represent a pure quantum high-spin state with multiple spin-1/2 states, and has later been extended to describe Hermitian multiband topological systems. For a spin-\( L \) state (\( \Phi \)) which has \( 2L+1 \) components, it can be expressed in terms of \( 2L \) spin-1/2 states according to the Schwinger boson representation theory:
\[
|\Phi\rangle = \frac{1}{2NL} \prod_{l=1}^{2L} (\cos(\frac{\theta_l}{2})a^\dagger_l + \sin(\frac{\theta_l}{2})e^{i\phi_l}a_l^\dagger)|0\rangle.
\]

Hence, a spin-\( L \) state can be decomposed to \( 2L \) spin-1/2 states by finding the roots of the following MSR equation:
\[
\sum_{l=0}^{2L} (-1)^l C_{2L-l+1} x^{2L-l} = 0,
\]

where \( C_\alpha \) denotes the wavefunction components of a spin-\( L \) state with \( \alpha \in \{1, 2, ..., 2L + 1\} \), and \( x_l \) being the found MS solutions.

In non-Hermitian \( J \)-band systems, the \( m \)-th right eigenstate of the system has \( J \) components in which each component can be understood as \( C_{m,l} \), i.e. \( \psi_{R,m}(k) = (C_{m,1}, C_{m,2}, ..., C_{m,J})^T \). Therefore, the \( m \)-th right eigenstate is mapped to the spin-\( L \) state by considering \( 2L + 1 = J \). Further, the decomposition to MSRs can also be done for the right eigenstates by using the MSR equation Eq. (6), upon changing \( 2L \) to \( J - 1 \) in the equation.

Since the decomposition is done for a given band \( m \) and given wavenumber \( k \), we denote the roots of the equation to be \( x_{m,l}(k) \) as shown in the following sections. Of particular importance is that in non-Hermitian systems, an isolated edge state may correspond to the coalescence of multiple eigenstates. We find that the winding number thus defined summed over all energy bands satisfy the following relation:
\[
\sum_m \nu_m = \sum_r D_r,
\]

where \( D_r \) being the number of eigenstates under the open boundary condition (OBC) that coalesce into the \( r \)-th isolated edge state, dubbed as a \( D_r \)-fold coalescent edge state hereafter. Note however, in a finite-size system under OBC, a \( D_r \)-fold coalescent edge state will be de-coalescent into totally \( D_r \) edge states with slightly different eigenenergies and spatial distributions, with the total number of such edge states still directly given by \( \sum_m \nu_m \).

Before moving on to the next section, we stress that we have only applied the MSR to right eigenstates in the above discussions. We have checked that using left eigenstates will yield the same conclusions.
IV. THE BULK-BOUNDARY CORRESPONDENCE

In a Hermitian 1D system, there is the bulk-boundary correspondence between the Zak phase evaluated under PBC and the number of edge states of the system under OBC. In this section, we will show that the winding number of the MSs, as defined above, can help characterize the number of isolated edge states in non-Hermitian multiband systems, even when EPs are present in the band structure and the Zak phase is ill-defined. For the rest of this paper, we consider the model of Eq. (1) with \( J = 3, 4 \) as representative examples, with more demonstrations with larger \( J \), i.e. \( J = 5 \), are shown in Appendix B.

A. Reciprocal system with separable bands

We first consider a reciprocal system with \( \delta_j = 0 \) for \( j \in \{1, 2, 3\} \), and non-Hermiticity is introduced solely from the imaginary on-site potential. In Fig. 2 we illustrate the PBC and OBC spectra for two typical cases with and without edge states isolated from the three separable continuous bands.

![Image of energy spectra for trivial and non-trivial cases](image)

**FIG. 2:** (a) and (b) respectively show the energy spectra of the topologically trivial case \((t_3 = 0.1)\) and non-trivial case \((t_3 = 0.9)\). The purple circles indicate the energy spectrum under OBC, and the red, blue, and green curves indicate the three energy bands of the system under PBC. Parameters for both cases: \( N = 120, t_1 = t_2 = \sqrt{2}/2, \mu_1 = \sqrt{2}, \mu_2 = 0, \mu_3 = -\sqrt{2}, \delta_j = 0 \) for \( j \in \{1, 2, 3\} \). Insets show the real space distributions \( \rho_{j,n} = |\psi_{j,n}|^2 \) of the two-fold coalescent edge states, with \( \psi_{j,n} \) being the amplitude of their wavefunctions at lattice site \((j,n)\).

In both cases, the PBC spectrum follows well with the OBC spectrum, suggesting the absence of NHSE. Thus bulk-boundary correspondence between the PBC system and isolated edge states under OBCs is expected to hold. Indeed, for the case of Fig. 2(a) without any isolated edge state, it is found that the trajectories of MSs for each band do not enclose the z-axis [Fig. 3(a)], meaning that the winding number takes \( \nu_m = 0 \) for \( m = 1, 2, 3 \). On the other hand, MSs for two of the three bands in Fig. 2(b) wind around the z-axis, indicating a nontrivial topology and corresponding edge states of the system. Note that in most cases, the trajectories of a pair of MSs for a single band exchange with each other as \( k \) varies from 0 to \( 2\pi \), and go back to themselves at \( k = 4\pi \). In such cases, the winding number \( \nu_m \) defined as summation over all MSs for the \( m \)th band is equivalent to the total winding of one of the MSs with \( k \) varying from 0 to \( 4\pi \).

In Fig. 2 we further illustrate the azimuthal angle \( \phi_m \) for each MS as a function of \( k \). We can see that for band 1 (blue) and band 3 (red) of the topologically nontrivial case, \( \phi \) changes by \( 4\pi \) as \( k \) goes through the BZ twice, corresponding to winding numbers \( \nu_{1,3} = 2 \). On the other hand, the second band in the same case has a winding number of \( \nu_2 = 0 \), which is the same for any band in the topologically trivial case in Fig. 2(a). The total winding number of the nontrivial case is hence given by

\[
\sum_m \nu_m = 4,
\]

which agrees with the fact that we obtain two two-fold coalescent edge states isolated from the continuous bands in Fig. 2(b).

Finally, to understand if our proposed topological characterization at least covers the traditional Zak phase based approach, we inspect the associated Zak phases by use of Eq. (4) for a comparison. Numerically, we obtain \( \gamma^{(1,2,3)} = (0.0035, -0.0035, 0)\pi \) for the topologically trivial case in Fig. 2(a), and \((0.1671, 3.8329, 0)\pi \) for the topologically nontrivial case in Fig. 2(b). Note that the Zak phases are not quantized for each individual band here, because the system we have chosen does not possess chiral symmetry nor inversion symmetry that protects a quantized Zak phase. Nevertheless, it has been shown that in Hermitian cases, the number of edge states can be related to the summation of Zak phases of all energy bands. Consistent with this, we respectively obtain \( \sum_m \gamma^{(m)} = 0 \) and \( 4\pi \) for the two cases here, which are in agreement with our defined winding number and the number of two-fold coalescent edge states. This being the case, for the examples here our approach does not outperform the Zak phase approach yet.
B. Inseparable bands with EPs

Since the energy spectrum of a non-Hermitian system is complex in general, EPs can exist when different energy bands at the same quasi-momentum $k$ coincide on the complex energy plane. In the presence of EPs, the eigenstates of these bands coalesce into one, leading to an incomplete Hilbert space and a non-diagonalizable Hamiltonian. Such situations are of more interest to us, because the Zak phase cannot be properly defined for each individual band. The central question is then the following: in such cases with EPs, can our defined winding numbers be used to predict the number of edge modes isolated from continuous bands on the complex energy plane?

In Fig. 5, the three energy bands coalesce at zero energy when $k = \pm \pi/2$, and two two-fold coalescent edge states exist, well separated from the continuous bands along the imaginary axis. To see the topological origin of these coalescent edge states, we plot the three bands by three different colors in Fig. 5 and then inspect the trajectories of their associated MSs of each band in Fig. 6. It is found that the first two bands give winding numbers $\nu_m = 1$, and the third band gives $\nu_m = 2$. Collectively, the summation of the winding number agrees with the summed total number of all coalescence edge states. By contrast, the calculated Zak phase summed over all energy bands for the situation here with EPs does not give a quantized value. Clearly then, our topological characterization prevails but the Zak phase approach breaks down. As a side note, it is not always straightforward to directly observe the winding from the trajectories of MSs on the Bloch sphere, especially when the system has many bands (see Appendix B 2). Therefore, a numerical calculation through Eq. (7) should always be done to obtain the winding number.
FIG. 5: Purple circles show the energy spectrum under OBC, and the red, green and blue curves show the energy spectrum of the 3 bands under PBC. All three bands coincide with each other at energy 0, causing an EP in the system. Parameters are $N = 120$, $t_1 = t_2 = \sqrt{2}/2$, $t_3 = 1$, $\mu_1 = \sqrt{2}$, $\mu_2 = 0$, $\mu_3 = -\sqrt{2}$ and $\delta_j = 0$.

To further illustrate the power of our method, we provide a phase diagram by evaluating the summed winding number of MSs of the system with varying parameters $t_1 = t_2$ and $t_3$, as shown in Fig. 7 with different winding numbers represented by different colors. The region where one or more EPs presents is enclosed by solid black curves, which are obtained from [See Appendix C]

$$2t_1^2 + t_3^2 - 2 = 0,$$

$$\sqrt{\frac{2t_1^2 + t_3^2 - 2}{3}} \frac{1}{t_1 t_3} = 1,$$  \hspace{1cm} (10)

corresponding to the ellipse curve and the two almost straight lines in Fig. 7 respectively. Across these lines, the number of EPs of the continuous bands changes between zero and nonzero, representing an EP phase transition. In the absence of EP, the summed winding number agrees with the summed Zak phase (divided by $\pi$), as we have discussed in Sec. IV A. When EPs present, the Zak phase is ill-defined but we can still use the summed winding number as a topology invariant to characterize the number of isolated edge states. Note that there is a clear transition line (yellow) inside the region with the presence of EPs. Such a region with EPs is usually considered as a critical region lying between different topological phases. Interestingly, our results indicate that within such a critical region with EPs, there is a further boundary separating different topological phases. This transition is unique in non-Hermitian systems, as edge states may be isolated from inseparable continuous bands only when they possess complex energies.

C. The presence of NHSE

Although NHSE is absent in our previous examples, it plays a crucial role in many non-Hermitian systems and can greatly affect our understanding of their topological properties. With the presence of NHSE, bulk-boundary correspondence breaks down, and the energy spectrum under PBCs and OBCs behaves completely different. Therefore, we cannot directly apply the MSR method to the PBCs system and calculate the winding number to characterize isolated edge states under OBCs in this case.

To recover the bulk-boundary correspondence, we need to consider the so-called non-Bloch Hamiltonian $\tilde{h}(k) = h(k + ik)$ such that for a certain $\kappa$, the energy spectrum of $\tilde{h}(k)$ does not form loops and reproduce OBC spectrum in the complex plane. Therefore, the procedure to deal with a non-Hermitian system typically consists of the following steps in general:

FIG. 6: (a-c) MSR for each of the three bands, corresponding to $\nu_{1,2,3} = (1,1,2)$ respectively. (d) the MSR of all energy bands, where two EPs are marked with light blue dots.
FIG. 7: The phase diagram obtained by varying the parameters $t_1 = t_2$ and $t_3$. The other parameters remain unchanged, as in the previous example in Fig. 5. The winding numbers in different regions are labeled in the figure. Topological transitions occur when parameters vary across the yellow lines separating regions with different winding numbers. EP phase transitions are given by the black solid lines, and the system possesses one or more EPs of continuous bands in the region enclosed by these black lines.

(i) Obtain the Bloch Hamiltonian of the system.
(ii) Calculate the energy spectrum as well as the eigenstates.
(iii) Check the PBC energy spectrum. If it forms loops, we need to calculate the $\kappa$ and obtain the non-Bloch Hamiltonian, then we redo the second step. If not, we can proceed to the next step.
(iv) Solve the MSR equation (6) and calculate the azimuthal angle of $\phi_{m,l}$.
(v) Calculate the winding number of MSs, which can then be used to indicate the number of isolated edge states of the system.

In Fig. 8a we illustrate an example with the presence of both NHSE and edge states isolated from the continuous OBC band. Numerically, we find that the non-Bloch Hamiltonian reproduces the OBC spectrum (except for isolated edge states) at $\kappa \sim 2.67$ [Fig. 8b], and bulk-boundary correspondence is expected to be restored. We then calculate the MSR for the non-Bloch Hamiltonian, and the results are shown in Fig. 9. Both the summed winding number and the summed Zak phase are 4, in agreement with the fact that there are two two-fold coalescent edge states in this case. Therefore, the bulk-boundary correspondence is fully recovered and our characterization with the winding number of the MSs remains valid for the non-Bloch Hamiltonian.

FIG. 8: The energy spectra of both PBC and OBC for the Bloch Hamiltonian and non-Bloch Hamiltonian, respectively. Purple circles indicate the energy under OBC, and the red, green and blue curves show the energy under PBC. Energy spectrum under PBC in (a) forms a loop, showing the presence of the skin effect. With $\kappa = 2.67$, the energy spectrum of the non-Bloch Hamiltonian under PBC does not form a loop, showing that it is free from the skin effect. Other parameters for both cases are $N = 120$, $t_1 = t_2 = 0.4$, $t_3 = 1.2$, $\delta_1 = \delta_2 = 0.2$, $\delta_3 = 1.1$ and $\mu_j = 0$.

D. 4-band system with 3 isolated edge states

Besides the cases with EPs, let us examine a case where the system has an odd number of isolated edge states, a situation that can never be connected with the Zak phase. In particular, we consider below a 4-band case from our model with $J = 4$, and in certain parameter regime, this case yields three non-coalescent edge states isolated from the continuous bands, as shown in Fig. 10a. NHSE also presents in this case as the PBC Bloch bands form some closed loops and are distinguished from the OBC bands. Numerically, we obtain $\kappa \sim 0.75$ for the non-Bloch Hamiltonian to recover the OBC spectrum, which is illustrated in Fig. 10b.
FIG. 9: The three images in (a) and (b) are corresponding to the three bands (red, blue, and green in Fig. 8b respectively). The two colors in each plot here indicate the two MSs for a given band. Their winding number are 1, 2, 1 respectively.

By applying Eq. (6), we obtain the corresponding MSRs, and the obtained results are shown in Fig. 11. It is seen that the winding number is $\nu_m = 1$ for $m = 1, 2, 3$, and 0 for $m = 4$. This observation is also verified by our direct numerical approach to $\nu_m$. Thus the summation of the winding numbers reflects the total number of isolated edge states in this case.

Remarkably, the Zak phases summed over all energy bands of non-Bloch Hamiltonian may quantize to an odd multiple of $\pi$ only when the system goes around an exceptional degeneracy as we scan $k$ from 0 to $2\pi$, the precise situation where the system must have NHSE. However, by construction the NHSE has been “removed” from the non-Bloch Hamiltonian through the complex deformation $k \rightarrow k + i\kappa$. That is, the summed Zak phase can only take an even multiple of $\pi$ for a non-Bloch Hamiltonian, hence cannot reflect the number of isolated edge states in this case. Indeed, numerically, we obtain $\gamma^{(1,2,3,4)} = (1.0128, 1.9608, 1.0128, 0.0136)\pi$, which sum to a quantized value of 4$\pi$, but our system has only three edge states! We have thus demonstrated again that our topological characterization is superior to the Zak phase approach.

FIG. 10: (a) and (b) show the energy spectra of the Bloch Hamiltonian and non-Bloch Hamiltonian respectively. The $\kappa$ of the non-Bloch Hamiltonian is found to be 0.75. Parameters are $t_1 = 1$, $t_2 = 0.8$, $t_3 = 1$, $t_4 = 1.2$, $\delta_1 = 0.2$, $\delta_2 = 1.7$, $\delta_3 = 0.2$, $\delta_4 = 0.2$, $\mu_1 = 0.5$, $\mu_2 = -0.3$, $\mu_3 = 0.4$, $\mu_4 = 0.9$.

V. CONCLUSIONS

In summary, we have used the MSRs to decompose the eigenstates of a non-Hermitian multiband system such that we can visualize them on the Bloch sphere. We have proposed a winding number of the MSs as a new topological invariant. Our defined topological invariant successfully characterizes the number of isolated edge states of non-Hermitian multiband systems under OBC. As a marked result, our topological characterization is effective even in the presence of EPs. Indeed, the winding numbers of the MSs are more generally applicable than the Zak phase, with the latter being ill-defined as the Hamiltonian becomes non-diagonalizable. Via our proposed topological invariant, we are able to predict the change in the number of isolated edge states and hence identify topological transitions in a parameter region where EPs are present and the band are inseparable. We have further applied our method to examples with non-Hermitian skin effects, and again verified that the bulk-boundary correspondence between the isolated edge states and the topological invariant we define can be restored by considering a non-Bloch Hamiltonian, obtained by a complex shifting of the quasi-momentum. Along this line, we have also discussed an example with an odd number of isolated edge states, where the Zak phase necessarily fails to predict the number of isolated edge states, whereas our topological invariant again agrees with the number of edge states. Such extraordinarily wide applicability of our approach may trigger further studies and bring us more insights into the interplay between exceptional degeneracies and
topological properties.

FIG. 11: The MSR of the 4 bands. (a-c) correspond to the 3 band on top in Fig. 10b, and the bottom right correspond to the 1 band at the bottom in Fig. 10b. Their winding numbers are 1, 1, 1, 0 respectively.

Note added. During the final stage of our manuscript preparation, we became aware of a preprint, which uses MSRs to study a three-band non-Hermitian Lieb lattice model, with a very different focus.

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Appendix

Appendix A: Non-Hermitian Zak phase and the winding number of the right or left eigenstates for two-band systems

A two-band non-Hermitian system can be described by the Hamiltonian

$$H = \sum_k h_x(k)\sigma_x + h_y(k)\sigma_y + h_z(k)\sigma_z + h_0(k)I, \quad (A1)$$

with $\sigma_{x,y,z}$ the Pauli matrices acting on a pseudospin-1/2 space, and $I$ the corresponding $2 \times 2$ identity matrix. Its left and right eigenstates are given by

$$|\psi_R^+\rangle = \left(e^{-i\phi}\cos\frac{\theta}{2} \sin\frac{\theta}{2}\right), \quad |\psi_R^-\rangle = \left(-e^{-i\phi}\sin\frac{\theta}{2} \cos\frac{\theta}{2}\right), \quad (A2)$$

and

$$|\psi_L^+\rangle = \left(e^{i\phi}\cos\frac{\theta}{2} \sin\frac{\theta}{2}\right)^T, \quad |\psi_L^-\rangle = \left(-e^{i\phi}\sin\frac{\theta}{2} \cos\frac{\theta}{2}\right)^T, \quad (A3)$$

with $\cos \theta = h_z/\sqrt{h_x^2 + h_y^2 + h_z^2}$ and $\cos \phi = h_x/\sqrt{h_x^2 + h_y^2}$, and $\pm$ denoting the two bands. Note that we have omitted the dependence of $k$ for simplicity. Without loss of generality, we consider the Zak phase of the lower band, which is given by

$$\gamma = \text{Re} \oint_{BZ} \frac{\partial \phi}{\partial k} \sin^2 \frac{\theta}{2} \, dk. \quad (A4)$$

In Hermitian systems with a chiral symmetry $\sigma_z h(k)\sigma_z = -h(k)$, we have $\theta = 0$, and the Zak phase is given by half of the winding angle of $\phi$ throughout Brillouin zone, corresponding to a quantized winding number. Degenerate topological edge states exist whenever the winding angle is nonzero. In the absence of a chiral symmetry (and other symmetries that protect 1D topology), the degeneracy of edge states will be lifted, and they are no longer protected by topology. Nevertheless, the existence of these edge states can still be characterized by the winding number of the phase angle $\phi$, which indicates a topological origin of them despite the lack of topological protection.

For non-Hermitian systems, both angle parameters take complex values in general, thus we rewrite them as $\phi = \phi_r + i\phi_i$ and $\theta = \theta_r + i\theta_i$, with $\phi_r,i$ and $\theta_{r,i}$ being real. Nevertheless, due to the periodicity of the Brillouin zone, imaginary phase factors $\theta_i$ and $\phi_i$ must go back to their original values when $k$ varies a period, and so does $\theta_r$ as it is originated from the altitude angle in the Hermitian limit. Therefore the winding corresponding to the Zak phase is solely given by the winding of $\phi_r$.

In the main text, we have applied MSR on the right eigenstates only, containing no information of the left
eigenstates. In the simplest two-band picture, each band consists of only one MS, directly given by the right eigenstates. Therefore we shall rewrite the right eigenstates with the orthogonal normalization condition, which yields

\[ |\psi'_+\rangle = \left( e^{-i\phi' \cos \frac{\theta'}{2}} \sin \frac{\theta'}{2} \right), \quad |\psi'_-\rangle = \left( e^{-i\phi' \sin \frac{\theta'}{2}} - \cos \frac{\theta'}{2} \right) \]  

(A5)

with \( \phi' \) and \( \theta' \) being real phase parameters. \( |\psi'_\pm\rangle \) and \( |\psi^R\pm\rangle \) shall be equivalent up to an overall coefficient. Taking the eigenstates of “−” band as an example, requiring \( |\psi'_{-}\rangle = c_- |\psi^R_{-}\rangle \) with \( c_- \) a coefficient, it is straightforward to obtain

\[
e^{-i\phi'} = e^{-i(\phi_r + \pi/2)} e^{i\phi_r c_- (e^{-\frac{\theta_r}{2}} e^{i\frac{\theta_r}{2}} - e^{\frac{\theta_r}{2}} e^{-i\frac{\theta_r}{2}})},
\]

\[
\cos \frac{\theta'}{2} = \frac{c_-}{2} (e^{-\frac{\theta_r}{2}} e^{i\frac{\theta_r}{2}} + e^{\frac{\theta_r}{2}} e^{-i\frac{\theta_r}{2}}). \tag{A6}
\]

We can see that for each individual point in the Brillouin zone, \( \phi' \) is given by \( \phi_r \) plus \( \pi/2 \) and some phases given by \( c_- \) and \( \theta_i, r \). However, neither of these extra phases may yield a nonzero winding over a period, as \( c_- \) depends only on \( \theta_i, r \), which must go back to themselves as discussed earlier. Therefore, with \( k \) varying from 0 to \( 2\pi \), \( \phi' \) and \( \phi_r \) must give the same winding number, reflecting the number of isolated edge states as demonstrated in the main text. Finally, we note that though we have only considered the right eigenstates in above discussion, this analysis also applies to left eigenstates.

Appendix B: Examples in 5-band systems

MSR can also be applied to multiband systems with even more bands. Here, we provide two examples with separable bands and inseparable bands in a 5-band system that is free from the skin effect (i.e. \( \delta_j = 0 \) for \( j \in \{1, 2, 3, 4, 5\} \)).

1. Separable bands

Considering the parameters as follow: \( t_1 = t_4 = 2 \), \( t_2 = t_3 = \sqrt{6}/2 \), \( t_5 = 0.9 \), \( \mu_1 = -\mu_5 = 4 \), \( \mu_2 = -\mu_4 = 2 \), \( \mu_3 = 0 \) and \( \delta_j = 0 \). Insets show the real space distribution of the edge states.

We can see that for each individual point in the Brillouin zone, \( \phi' \) is given by \( \phi_r \) plus \( \pi/2 \) and some phases given by \( c_- \) and \( \theta_i, r \). However, neither of these extra phases may yield a nonzero winding over a period, as \( c_- \) depends only on \( \theta_i, r \), which must go back to themselves as discussed earlier. Therefore, with \( k \) varying from 0 to \( 2\pi \), \( \phi' \) and \( \phi_r \) must give the same winding number, reflecting the number of isolated edge states as demonstrated in the main text. Finally, we note that though we have only considered the right eigenstates in above discussion, this analysis also applies to left eigenstates.

FIG. 12: Black circles show the energy spectrum under OBC, and the red, green, blue, orange and purple curves show the energy spectrum of the 5 bands under PBC. Parameters are \( N = 200 \), \( t_1 = t_4 = 2 \), \( t_2 = t_3 = \sqrt{6}/2 \), \( t_5 = 0.9 \), \( \mu_1 = -\mu_5 = 4 \), \( \mu_2 = -\mu_4 = 2 \), \( \mu_3 = 0 \) and \( \delta_j = 0 \). Insets show the real space distribution of the edge states.

Four non-coalescent edge states isolated from the continuous bands can be observed in the energy spectrum of Fig. 12. By obtaining the MSR of this model and plotting the stars on the Bloch sphere, we can also observe that the winding number is \( \nu_m = 1 \) for \( m = 1, 2, 4, 5 \) and \( \nu_3 = 0 \), as shown in Fig. 13.

FIG. 13: The MSR of all bands are combined in the same Bloch sphere, in which the colors are corresponding to the energy bands in Fig 12.
2. Inseparable bands with EPs

Considering $t_5 = 6$ and the rest of the parameters remains the same as in the previous section. The energy spectrum is shown in Fig. 14. There are also 4 isolating edge states in this case as shown in the figure. Note that the two bands with $m = 1, 2$ (blue,red) are pinned at two points on the complex energy plane, corresponding to two flat bands throughout the BZ.

![FIG. 14: Black circles show the energy spectrum under OBC, and the red, green, blue, orange and purple curves show the energy spectrum of the 5 bands under PBC. Parameters are $N = 200, t_1 = t_4 = 2, t_2 = t_3 = \sqrt{5}/2, t_5 = 6, \mu_1 = -\mu_5 = 4, \mu_2 = -\mu_4 = 2, \mu_3 = 0$ and $\delta_j = 0$. Insets show the real space distribution of the edge states.](image)

However, if we solve the MSR and plot it in the Bloch sphere, the stars are rather messy in this case, as shown in Fig. 15. It is hard to directly obtain the winding information from the plot in higher multiband systems with the presence of EPs. Nevertheless, the winding numbers can still be obtained numerically through Eq. (C1). In this specific example, the winding numbers are $\nu_m = 0$ for $m = 1, 2, \nu_m = 1$ for $m = 4, 5$, and $\nu_3 = 2$.

![FIG. 15: The MSR of all bands are combined in the same Bloch sphere, in which the colors are corresponding to the energy bands in Fig. 14.](image)

Appendix C: solutions of EP phase boundaries

The eigenenergies of our system under PBC can be obtained from the eigenequation $\det[h(k) - E_k] = 0$ of Eq. (2) in the main text, yielding

$$E_k^3 - (2t_1^2 + t_3^2 - 2)E_k - 2t_1^2 t_3 \cos k = 0 \quad (C1)$$

for the parameters we considered in Fig. 7. In the presence of EPs, this equation can be written as $(E_k - E_1)^2(E_k - E_2) = 0$. Compared with the coefficients of Eq. (C1), we have

$$3E_1^2 = 2t_1^2 + t_3^2 - 2, \quad (C2)$$
$$E_1^3 = -t_1^2 t_3 \cos k. \quad (C3)$$

Therefore, to have a real solution of $k$ (and hence EPs in the BZ), $-E_1^3/t_1^2 t_3$ must takes a real value between $-1$ and $1$, and we can obtain the following two conditions:

$$2t_1^2 + t_3^2 - 2 \geq 0 \quad (C4)$$

to give a real value of $E_1$, and

$$| \cos k | = \sqrt{\frac{2t_1^2 + t_3^2 - 2}{3} \frac{1}{t_1^2 t_3}} \leq 1. \quad (C5)$$

Thus the EP phase boundaries in Fig. 7 is obtained when the above inequalities takes the equal sign, i.e. Eqs. (10) in the main text.
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