Homotopical classification of non-Hermitian band structures

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We proposed a framework towards the topological classification of non-Hermitian band structures. Different from previous $K$-theoretical approaches, our approach is homotopical, which enables us to see more topological invariants. Specifically, we considered the classification of non-Hermitian systems with separable band structures. We found that the whole classification set is decomposed into several sectors, based on the braiding of energy levels. Each sector can be further classified based on the topology of eigenstates (wave functions). Due to the interplay between energy level braiding and eigenstates topology, we found some torsion invariants, which only appear in the non-Hermitian world. We further proved that these new topological invariants are unstable, in the sense that adding more bands will trivialize these invariants.

I. INTRODUCTION

While we are used to assuming the Hermiticity of Hamiltonians, as required by the axioms of quantum mechanics, there has been growing interest in non-Hermitian Hamiltonians these years. Indeed, in the Hermitian quantum mechanics framework, non-Hermitian Hamiltonian can emerge as an effective description of open system with gain and loss [1–21] or systems with finite-lifetime quasiparticles/non-Hermitian self energy [22–24], which can be experimental realized in atomic or optical systems [25–31]. Moreover, non-Hermitian Hamiltonians with certain properties can serve as an extension of conventional Hermitian quantum mechanics [32–34].

Classification of topological phases of matter is one of the central problems in condensed matter physics for the last two decades. While a complete classification of topological phases is still in progress, the classification for gapped non-interacting fermions is well-established [35–37] based on the geometry and topology of the band structures.

Inspired by the great success in topological phases for Hermitian systems, there has been lots of works focusing on the topological aspects of non-Hermitian systems. On the one hand, many familiar constructions for topological phases can be extended in the case of non-Hermiticity. For example, people have constructed the non-hermitian counterparts for Su-Schrieffer-Heeger model [5, 20, 38–41], Chern insulators [42–46], and quantum spin hall effects [47]. On the other hand, non-Hermitian systems also exhibit many unusual phenomena with no counterpart in the Hermitian world. These include exceptional points [48–50], anomalous bulk-edge correspondence [20, 51–54], non-Hermitian skin effect [42, 55] and sensitivity to boundary conditions [51, 56]. For a recent review, see Ref. 57 and references therein.

There has also been some works [58–62] on the general classification of non-Hermitian systems, aiming at a generalization of the Hermitian periodicity table [36, 37]. In these works, the authors first determined reasonable symmetry classes in the non-Hermitian setting (a generalization of Ref. 35), then use a unitarization/Hermitianization map to reduce the problem into the Hermitian setting where one can apply $K$-theory.

In this paper, we proposed a more conceptually straightforward homotopical [63–66] framework towards the topological classification of non-Hermitian band structures, which enables us to see more topological invariants beyond $K$-theoretical approaches. With rigorous algebraic-topological calculation, we implemented our idea in detail for systems with no symmetry.

We found that, due to the non-Hermiticity of the Hamiltonian, energies can be complex and therefore braids with each other in the complex plane, which decomposed the whole classification set into several braiding sectors. Each sector can be further classified based on the topology of eigenstates (wave functions), akin to the usual topological classification for Hermitian systems, however with more subtitles coming from the braiding of energy levels and the shape of the Brillouin zone (torus vs. sphere). We found some new torsion invariants (for example, $\mathbb{Z}_2$), and a physical explanation of these new invariants is given.

We also considered the stability of these new invariants, in the sense that whether adding other bands will trivialize these invariants, even if the band has no crossing with previous bands. Similar to the $\mathbb{Z}$ invariants of Hopf insulators [67], our torsion invariants are unstable. We managed to give a combinatorial proof for instability in general. The physical origin of the instability is also discussed.

This paper is organized as follows. In Sec. II, we discuss our classification principle: what kind of systems we are looking at, and what we mean by two systems are looking at, and what we mean by two systems are in the same class. In Sec. III, the classification principle is implemented mathematically, and some examples are discussed in Sec. IV. Finally, we investigate the instability in Sec. V.

II. PRINCIPLE OF CLASSIFICATION

A classification problem, formally speaking, is to classify elements of a set according to some equivalence re-
lations. In many problems of condensed matter physics, the set is usually taken to be the set of Hamiltonians \( H \) with a “energy gap”, and \( H_1 \) and \( H_2 \) are equivalent if and only if they can be continuously connected while keeping the gap open.

For Hermitian systems, there is no subtlety regarding the meaning of the gap, since all eigenvalues of a Hermitian Hamiltonian are real and the meaning of a gap on the real line is clear. For non-Hermitian systems (interacting or not), however, the eigenvalues can be complex. Therefore, the meaning of a “gap” need to be further clarified [45, 59, 68].

Consider a non-interacting non-Hermitian system with translational invariance. Standard second quantization and band theory give rise to momentum-dependent one-body Hamiltonians \( H(k) \). In this paper, we will call \( \{ H(k) \} \) (\( k \in \text{BZ} \)), the Brillouin zone) a band structure, which contains information of both their spectrum \( E_i(k) \) and associated eigenstates \( |\psi_i(k)\rangle \).

One has at least the following different notions of the gap:

- **line gap** [59, 69]. There exists a (maybe curved) line \( l \) in the complex energy plane which separates the plane into two disconnected pieces. We require \( E_i(k) \neq l \) for all \( i \) and \( k \), and both connected components have some spectral points in them.

- **point gap** [58–60, 62]. \( E_i(k) \neq 0 \) for all \( i \) and \( k \). Here, 0 is a reference point which can be altered to any \( E_0 \).

- **separable band** [43, 45]. A specific band \( E_i(k) \) is called separable if \( E_j(k) \neq E_i(k) \) for all \( j \neq i \) and \( k \).

- **isolated band** [45]. A specific band \( E_i(k) \) is called isolated if \( E_j(k') \neq E_i(k) \) for all \( j \neq i \) and \( k, k' \).

Note that these notions are not mutually exclusive. For example, an isolated band is always separable; systems with isolated bands always have line gaps and hence always have point gaps. Also note that, the first two notions are applicable to general non-Hermitian systems, while the last two notions are specific to translational-invariant non-interacting cases by definition.

In our paper, we will consider the classification of separable band structures, since other cases were solved [58–62] by mapping back to the Hermitian case. However, there is one more problem with the definition of separability that needs to be discussed: the above mentioned \( E_i(k) \) may not be a well-defined function of \( k \).

For example, consider a one-dimensional systems with two bands, satisfying \( E_1(k) \neq E_2(k) \) for all \( k \). It is possible that \( E_1(2\pi) = E_2(0) \): if one follow the spectrum when \( k \) goes around the Brillouin zone (a circle in this case) starting from \( E_1(0) \), one may go to \( E_2(0) \) instead of going back to \( E_1(0) \), see Fig. 1. In this case, the notation “\( E_i(k) \)” (and therefore its separability) for a specific \( i \) may not be well-defined. Instead, it is better to define separability in a global manner: for any \( k \), \( E_i(k) \) \( (i = 1, \ldots, n) \) are all different. This definition of separability automatically rules out exceptional points, i.e., \( H(k) \) is not diagonalizable under similarity transformations, since it requires (algebraically) degenerated spectra.

To summarize, we will consider the following problem: classify the band structure \( \{ H(k) \} \) where spectrum of \( H(k) \) are non-degenerated and \( \{ H_0(k) \} \) and \( \{ H_t(k) \} \) are equivalent if and only if they can be continuously connected by \( \{ H_t(k) \} \) for \( t \in [0,1] \) and the spectra of \( H_t(k) \) for any \( t \) and \( k \) are always non-degenerated.

### III. CLASSIFICATION

Let us consider the general problem of classifying band structures with \( n \) bands on a \( m \)-dimensional lattice. Denote

\[
X_n = \text{the space of } H(k).
\]

Namely, it is the space of \( n \times n \) matrices with non-degenerated spectrum. Here the Brillouin zone will be the \( m \)-dimensional torus \( T^m \). Mathematically speaking, we want to find the homotopy equivalent classes of non-based maps from the Brillouin zone \( T^m \) to \( X_n \), denoted by \( [T^m, X_n] \).

It will be important to distinguish \( T^m \) and \( S^m \), since they will give different answers. It is also important to distinguish based maps and non-based maps: the former requires a chosen point in \( T^m \) to be mapped to a chosen point in \( X_n \) while the latter has no such requirement.

To calculate the classification, we are going to use some standard methods in algebraic topology. For an introduction, see Ref. 70.

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1 On the other hand, for continuous systems the appropriate choice the based map from \( S^m \) to \( X_n \), since the Brillouin zone here is \( S^m \) with the requirement that infinite momentum maps to some fixed point [37].
A. The space $X_n$ and its homotopy groups

An element $H$ of $X_n$ is an $n \times n$ matrix with non-degenerated spectrum, which can be represented as $(\lambda_1, \ldots, \lambda_n, \alpha_1, \ldots, \alpha_n)$. Here, $(\lambda_1, \ldots, \lambda_n)$ are ordered eigenvalues satisfying $\lambda_i \neq \lambda_j$, i.e.,

$$(\lambda_1, \ldots, \lambda_n) \in \text{Conf}_n(\mathbb{C}),$$

where $\text{Conf}_n(\mathbb{C})$ is the configuration space of ordered $n$-tuples in $\mathbb{C}$. $(\alpha_1, \ldots, \alpha_n)$ are corresponding eigenvectors (up to complex scalar multiplications), which are linearly independent. Denote the space of linearly independent ordered $n$-vectors (up to scalar) in $\mathbb{C}^n$ as $F_n$. We have

$$F_n \cong \text{GL}(n)/\mathbb{C}^*,$$

since $\text{GL}(n)$ acts transitively on $F_n$ and the stabilizer group is $\mathbb{C}^*$, where $\mathbb{C}^* = \mathbb{C} - \{0\}$, the group of nonzero complex numbers. Another way to understand this equation is to consider the columns of a $\text{GL}(n)$ matrix, which are ordered $n$-vectors in $\mathbb{C}^n$, while “up to scalar” is taken care of by $n$ independent scalar multiplications $\mathbb{C}^*$. The space $F_n$ is actually homotopic to the full flag manifold of $\mathbb{C}^n$.

This representation has some redundancies: one can permute $(\lambda_i, \alpha_i)$ and get the same matrix $H$. Therefore,

$$X_n \cong (\text{Conf}_n \times F_n)/S_n,$$

where $S_n$ is the permutation group acting on $\text{Conf}_n \times F_n$ as simultaneous permutations of $(\lambda_i, \alpha_i)$.

Consider $\pi_1(\text{Conf}_n)$, whose elements are (equivalence classes of) paths in $\text{Conf}_n$, which correspond to some pure braiding of $n$ mutually different points in $\mathbb{C}$. Here, “pure” means each point goes back to itself after the braiding. This is true since we are considering ordered $n$-tuples. Therefore,

$$\pi_1(\text{Conf}_n) = \text{PB}_n,$$

where $\text{PB}_n$ is the pure braiding group of $n$ points [71, 72].

It turns out [73] that $\text{Conf}_n = K(\text{PB}_n, 1)$, the classifying space of the group $\text{PB}_n$. Therefore,

$$\pi_m(\text{Conf}_n) = 0, \quad m \geq 2.$$  \hspace{1cm} (6)

The homotopy groups $\pi_m(F_n)$ can be obtained by the long exact sequence of homotopy groups [70], based on the fibration Eq. (3). For $m = 1$, we have:

$$\pi_1(\mathbb{C}^*) \to \pi_1(\text{GL}(n)) \to \pi_1(F_n) \to \pi_0(\mathbb{C}^*) = 0.$$  \hspace{1cm} (7)

Here, $\pi_1(\mathbb{C}^*) = \mathbb{Z}$, $\pi_1(\text{GL}(n)) = \mathbb{Z}$, which is essentially the determinant. The map $\pi_1(\mathbb{C}^*) \to \pi_1(\text{GL}(n))$ is exactly summing over $n$ components in $\mathbb{Z}$, which is surjective. Therefore $\pi_1(F_n) = 0$. For $m = 2$, we have:

$$0 = \pi_2(\text{GL}(n)) \to \pi_2(F_n) \to \pi_1(\mathbb{C}^*) \to \pi_1(\text{GL}(n)).$$  \hspace{1cm} (8)

Therefore, $\pi_2(F_n)$, as the kernel, is represented by $n$ integers with summation equals 0:

$$\{(t_1, \cdots, t_n) \in \mathbb{Z}^n \mid \sum t_i = 0\},$$

which is isomorphic to $\mathbb{Z}^{n-1}$. This representation with $n$ integers will be useful later. For $m \geq 3$, we have

$$0 = \pi_m(\mathbb{C}^*) \to \pi_m(\text{GL}(n)) \to \pi_m(F_n) \to \pi_{m-1}(\mathbb{C}^*) = 0,$$

therefore $\pi_m(F_n) = \pi_m(\text{GL}(n)) = \pi_m(U(n))$.

To summarize, the result is as follows:

$$\pi_m(F_n) = \begin{cases} 0, & m = 1 \\ \mathbb{Z}^{n-1}, & m = 2 \\ \pi_m(U(n)), & m \geq 3 \end{cases}.$$  \hspace{1cm} (11)

Now consider the space $X_n$. According to Eq. (4) and the fact that $S_n$ is discrete, higher homotopy groups $\pi_m(X_n)$ are the same as those of $\text{Conf}_n \times F_n$, therefore the same as Eq. (11), due to the fact in Eq. (6).

For the fundamental group $\pi_1$, one can take advantage of the fact that $\pi_1(F_n) = 0$ and show that:

$$\pi_1(X_n) = \pi_1(\text{Conf}_n/S_n) = B_n.$$  \hspace{1cm} (12)

Here $S_n$ acts on $\text{Conf}_n$ by permutations, giving the configuration space $\text{Conf}_n/S_n$ of non-ordered $n$-tuples in $\mathbb{C}$, whose fundamental group is $B_n$, the braiding group including “non-pure” braidings.

This is because a loop in $X_n$ corresponds to a path $p(t) = (p_1(t), p_2(t))$ in $\text{Conf}_n \times F_n$ such that $p_1(1) = gp_1(0)$ and $p_2(1) = gp_2(0)$ for the same $g \in S_n$. Note that $g$ is uniquely determined by $p_1(1)$ (the initial point $(p_1(0), p_2(0))$ is a fixed lifting) and $F_n$ is simply connected, the path one-to-one (homotopically) corresponds to a path in $\text{Conf}_n$ with $p_1(1) = gp_1(0)$ and therefore a loop in $\text{Conf}_n/S_n$. A more algebraic proof is to note that the actions of $S_n$ on $\text{Conf}_n \times F_n$ and $\text{Conf}_n$ are consistent, which gives the following pullback:

$$\begin{array}{ccc} \text{Conf}_n \times F_n & \to & \text{Conf}_n \\ \downarrow & & \downarrow \\ X_n & \to & \text{Conf}_n/S_n \end{array}$$  \hspace{1cm} (13)

and then apply the homotopy exact sequence for this pullback square.

The appearance of braiding group $B_n$ is easy to understand. Consider a one-dimensional band structure and follow the evolution of spectrum $\{E_i\}$ along the Brillouin zone circle. Similar to $n = 2$ case in Sec. II as shown in Fig. 1, in general points in $\{E_i\}$ will braid with each other during this evolution and may become other points after one cycle. The evolution of $n$ disjoint points is topologically classified by the braiding group $B_n$. 
B. The set $[T^m, X_n]$

The equivalent classes $[T^m, X_n]$ is related but may not equal to the homotopy groups $\pi_m$, which is, by definition, $(S^m, X_n)$. Here, $(-, -)$ is used for based maps, while $[-, -]$ is used for non-based maps. In general, $[T, X]$ is just a set with no extra structures, even if $T$ is a sphere, in which case $(T, X)$ is exactly a homotopy group. The relation between $[T, X]$ and $(T, X)$ for general spaces $T$ and $X$ is as follows [70]: There is a right action of $\pi_1(X)$ on $(T, X)$, and $[T, X] \cong (T, X)/\pi_1(X)$, the orbit set of the action.

We will first calculate $(T^m, X_n)$ and then use the above connection to obtain $[T^m, X_n]$.

In the case $m = 1$, $\pi_1(X_n)$ acts on $(T^1, X_n) = \pi_1(X_n)$ by conjugate:

$$[f] \gamma = [\gamma^{-1} \circ f \circ \gamma],$$

therefore $[T^1, X_n]$ is the set of conjugacy classes of group $B_n$. Determine the conjugacy classes of braiding group $B_n$ is a difficult problem except $n \leq 2$.

In the case $m = 2$, the set $(T^2, X)$ is given by [76] (see also Appendix A 1):

$$\{(a, b) \in \pi_1(X)^2 | ab = ba \} \times \pi_2(X) / \{ t - t^a, t - t^b | t \in \pi_2 \},$$

where $t^a$ is the result of $a \in \pi_1(X)$ acting on $t \in \pi_2(X)$.

Note that this is a noncanonical identification. In our problem, the result is:

$$\bigcup_{a,b \in B_n \atop ab = ba} \mathbb{Z}^{n-1} / \{ t - t^a, t - t^b \} \cong \bigcup_{a,b \in B_n \atop ab = ba} Q(n, a, b).$$

In other words, the classification of based maps is decomposed into several sectors, denoted by a pair of commuting braiding $a, b \in B_n$; classification within each sector $(a, b)$ is given by the quotient $Q(n, a, b)$, a finite-generated abelian group, by identifying $t$ with $t^a$ and $t^b$.

Physically, the braiding $a$, $b$ is given by following two nontrivial circles $l_a, l_b$ in the Brillouin zone $T^2$. Since $l_a l_b l_a^{-1} l_b^{-1}$ is the boundary of the 2-cell of $T^2$, the corresponding braiding $aba^{-1}b^{-1}$ must be trivial, hence $ab = ba$. Fixing $a, b$, the map on the 2-cell is determined by $\pi_2(X_n) = \pi_2(F_n) = \mathbb{Z}^{n-1}$, which are essentially $(n - 1)$ Chern numbers, up to some ambiguities taken care of by the quotient.

The action $t \rightarrow t^a$ here is determined as follows. Recall Eq. (9) that $\pi_2(X_n) = \mathbb{Z}^{n-1}$ can be represented by $\{(t_1, \cdots, t_n) \in \mathbb{Z}^n | \sum t_i = 0 \}$. $a \in B_n$ induced a permutation $\hat{a}$ in $S_n$ by forgetting the braiding. Then $t^a$ is represented by a permutation of $(t_1, \cdots, t_n)$:

$$(t_1, \cdots, t_n) \mapsto (t_{a(1)}, \cdots, t_{a(n)}).$$

The proof of this statement is a bit technical. However, since it is the root of most novel classifications in this paper, we give a detailed proof in Appendix A 2.

Now consider the action of $\pi_1(X_n) = B_n$ on $(T^2, X_n)$. Pick $c \in B_n$, then $c$ act on $(a, b)$ by conjugate:

$$(a, b) \rightarrow (c^{-1}ac, c^{-1}bc).$$

The action of $c$ on $\bar{t} \in Q(n, a, b)$ is induced by the action of $\pi_1(X_n)$ on $\pi_2(X_n)$: under $c$, $t$ goes to $t^c$, $t^a$ goes to $t^ac$, therefore $t - t^a$ goes to $t^c - (t^c)^{-1}ac$, therefore the action of $c$ on $\bar{t} \in Q(n, a, b)$ is well-defined as $\bar{c} = \bar{t} \in Q(n, c^{-1}ac, c^{-1}bc)$. Note that $Q(n, a, b) \cong Q(n, c^{-1}ac, c^{-1}bc)$, due to fact that Eq. (16) and Eq. (17) only care about the permutation structure of $a, b$, which is invariant under conjugation. We finally get:

$$[T^2, X_n] = \bigcup_{(a,b) \in B_n \atop ab = ba} Q(n, a, b),$$

where $(a, b)$ means a conjugacy class of commuting pairs under Eq. (18), and $Q(n, a, b) = Q(n, a, b)/\pi_1(X_n)$ is the orbit set (not quotient group) of $Q(n, a, b)$ under the stabilizer subgroup $\pi_1(X_n)$ that keeps $(a, b)$ invariant.

The reason for the appearance of this $\pi_1(X_n)$ action can be traced back to the difference between $[T, X]$ and $(T, X)$. Physically, there is no natural way to label the bands (even if no braiding happens, namely, $a = b = id$). In the Hermitian case, bands are naturally ordered according to their energy, which is not the case for complex energy levels. Therefore there are some redundancies corresponds to change the label of bands (see Sec. IV B for an example). Also note that, while $Q(n, a, b)$ is a finite generated abelian group, $Q(n, a, b)$ is just a set.

IV. EXAMPLES

A. Non-Hermitian bands in one dimension

In the case of $m = 1$, we know from Sec. III B that band structures are classified by the conjugacy classes of group $B_n$.

Determine the conjugacy classes of braiding group $B_n$ is only easy when the number of bands $n = 2$, where the braiding group $B_2$ is just $\mathbb{Z}$: $a \in \mathbb{Z}$ is the number of elementary braiding (half of a $2\pi$ rotation), with $a$ even implies a pure braid and $a$ odd implies a permutation. In this case, each conjugacy class only has one element, since $\mathbb{Z}$ is abelian. Therefore, the classification is given by:

$$[T^1, X_2] = \mathbb{Z}. \quad (20)$$

Same classification was found in Ref. 20, 41, and 45. Note that some authors use $\frac{1}{2}\mathbb{Z}$ instead of $\mathbb{Z}$: their spectral "vorticity" is exactly one half of the above invariant.

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2 For a review of the conjugacy problem in braiding group, see Ref. 74. It relies on the “Garside structure” [75].

3 For a review of the centralizer problem in the braiding group, see Ref. 77. The result heavily depends on the geometry of braiding, namely, the Nielsen-Thurston classification [78].
B. Two-band Chern “insulators”

Consider the case with \(m = n = 2\), namely, band structures with two bands in two dimensional (2D) space. This corresponds to Chern insulators in the Hermitian case. However, it may not be a true insulator in the non-Hermitian case if there is no line gap (to place the chemical potential).

Let us calculate \(Q(2, a, b)\) and \(\overline{Q}(2, a, b)\), where \(a, b \in B_2 = \mathbb{Z}\). There are four cases, depending on the even/odd of \(a\) and \(b\).

- \(a, b\) even. Then \(t^a = t^b = t\), therefore \(Q(2, a, b) = \mathbb{Z}\). The action of \(c \in \pi_1(X_n)\) on \(Q(2, a, b)\) might be nontrivial: it acts as opposite if \(c\) is odd (see below), therefore \(Q(2, a, b) = \mathbb{N}\), the set of nonnegative integers.

- \(a\) even, \(b\) odd. Then \(t^a = t\) while \(t^b = -t\) in the sense that \((s, -s)^b = (-s, s)\). Therefore \(Q(2, a, b) = \langle (s, -s), (2s, -2s) \rangle \cong \mathbb{Z}_2\). The action of \(\pi_1(X_n)\) at most takes \((s, -s)\) to \((-s, s)\), which has no effects on \(\mathbb{Z}_2\), therefore \(Q(2, a, b) = \mathbb{Z}_2\).

- \(a\) odd, \(b\) even. Same as above.

- \(a, b\) odd. Then \(t^a = t^b = -t\), \(Q(2, a, b) = \overline{Q}(2, a, b) = \mathbb{Z}_2\).

Therefore, band structures are classified by

\[
\bigcup_{a,b \in \mathbb{N}} \mathbb{N} \text{ or } \mathbb{Z}_2.
\]

The \(\mathbb{N}\) classification (instead of \(\mathbb{Z}\)) comes from the fact that we have no natural way to identify “upper band” and “lower band” as in the Hermitian case, since there \(C\) is not naturally ordered as \(\mathbb{R}\). This new feature of non-Hermitian classification will disappear if, for example, we have a fixed line gap, the classification will go back to \(\mathbb{Z}\).

The \(\mathbb{Z}_2\) classification in some sectors is a more interesting new phenomenon. It comes from the interplay between spectrum braiding and eigenvector topology (Chern band). A heuristic physical picture is as follows. For example, consider the case of \(a\) odd and \(b\) even. In this case, the Brillouin zone is better considered as a torus with size \(4\pi \times 2\pi\): by gluing two cylinders along a direction we can get a double Brillouin zone on which the energy level braiding, the Brillouin zone is better considered as a torus with size \(4\pi \times 2\pi\).

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- \(a\) even, \(b\) odd. Then \(t^a = t\) while \(t^b = -t\) in the sense that \((s, -s)^b = (-s, s)\). Therefore \(Q(2, a, b) = \langle (s, -s), (2s, -2s) \rangle \cong \mathbb{Z}_2\). The action of \(\pi_1(X_n)\) at most takes \((s, -s)\) to \((-s, s)\), which has no effects on \(\mathbb{Z}_2\), therefore \(Q(2, a, b) = \mathbb{Z}_2\).

- \(a\) odd, \(b\) even. Same as above.

- \(a, b\) odd. Then \(t^a = t^b = -t\), \(Q(2, a, b) = \overline{Q}(2, a, b) = \mathbb{Z}_2\).

Therefore, band structures are classified by

\[
\bigcup_{a,b \in \mathbb{N}} \mathbb{N} \text{ or } \mathbb{Z}_2.
\]

The \(\mathbb{N}\) classification (instead of \(\mathbb{Z}\)) comes from the fact that we have no natural way to identify “upper band” and “lower band” as in the Hermitian case, since there \(C\) is not naturally ordered as \(\mathbb{R}\). This new feature of non-Hermitian classification will disappear if, for example, we have a fixed line gap, the classification will go back to \(\mathbb{Z}\).

The \(\mathbb{Z}_2\) classification in some sectors is a more interesting new phenomenon. It comes from the interplay between spectrum braiding and eigenvector topology (Chern band). A heuristic physical picture is as follows. For example, consider the case of \(a\) odd and \(b\) even. In this case, the Brillouin zone is better considered as a torus with size \(4\pi \times 2\pi\): by gluing two cylinders along a direction we can get a double Brillouin zone on which the energy level braiding, the Brillouin zone is better considered as a torus with size \(4\pi \times 2\pi\).

The conjugacy classes and commuting pairs are hard to describe if \(n > 2\). However, the quotient \(Q(n, a, b)\) for given braiding sector \((a, b)\) are not hard to calculate.

Recall from Eq. (17) that \(\pi_2(X_n) = \mathbb{Z}^{n-1}\). The conjugacy classes and commuting pairs can be calculated by

\[
\langle t - t' \rangle = \langle (t_1 - a_1), \ldots, t_n - t_n \rangle = 0.
\]

There are only \((n - 1)\) independent \(t_i\)'s: we can use \(t_n = -\sum_{i=1}^{n-1} t_i\) to get rid of the constraint. Then the

\[
\langle t - t' \rangle = \langle (t_1 - a_1), \ldots, t_{n-1} - a_{n-1} \rangle = 0.
\]
The subgroup Eq. (23) is generated by $2(n - 1)$ (not necessarily independent) generators. For example, take $t_1 = 1, t_2 = \ldots = t_{n-1} = 0, t_n = -1$ and consider the action of $a$, we get a generator $e_1 - e_1 - (i) - e_n + e_{a-1}(n)$, where $e_1 = (1,0,\ldots,0,-1), e_2 = (0,1,0,\ldots,0,-1), e_{n-1} = (0,\ldots,0,1,-1), e_n = (0,\ldots,0)$. Therefore, the $Q(n, a, b)$ is the quotient of $\langle e_1, \ldots, e_{n-1} \rangle$ with $2(n - 1)$ relations $e_i - e_{a-1}(i) - e_n + e_{a-1}(n) (i = 1, \ldots, n - 1)$. Its structure can be determined by standard procedure using Smith normal form.

As a simple example, consider the case where $a = 1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 1, b = 1 \rightarrow 4 \rightarrow 3 \rightarrow 2 \rightarrow 1$. This is possible, say, by taking $a$ to be a braiding with such permutation structure, then taking $b = a^{-1}$. The auxiliary “generators” given by $t_i = 1, t_1 = \ldots = t_{i-1} = t_{i+1} = \ldots = t_n = 0$ written in terms of $n$-tuples is the $i$th columns of the following matrix

$$
\begin{bmatrix}
1 & -1 & -1 \\
1 & 1 & -1 \\
-1 & 1 & 1
\end{bmatrix},
$$

(24)

Since the true generators are given by taking $t_i = 1, t_n = -1, t_j = 0 (j = 1, \ldots, i-1, i+1, \ldots, n-1)$, we need to subtract the last column from all other columns and delete the last row. The matrix of true generators for $\langle t - t^a \rangle$ is:

$$
\begin{bmatrix}
1 & -1 \\
1 & 1 \\
1 & 1
\end{bmatrix},
$$

(25)

and similarly for $b$:

$$
\begin{bmatrix}
2 & 1 & 1 \\
-1 & 1 & -1
\end{bmatrix}.
$$

(26)

Juxtapose those two matrices and calculate its Smith normal form, we get:

$$
\begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0
\end{bmatrix},
$$

(27)

which means $Q(4, a, b) = \mathbb{Z}_4$.

Another example is when $b = id$, i.e., no permutation. We can decompose $a$ into cycles: $a = (\ldots)\ldots(\ldots)$. Denote the length of each cycle to be $l_1, \ldots, l_k$ ($\sum_{i=1}^k l_i = n$) where $k$ is the number of cycles. In this case, we can follow the above procedure and get an explicit formula for $Q(n, a, b)$.

Denote an $l \times l$ matrix of form Eq. (24) to be $J_l$, then the counterpart of Eq. (24) by subtraction and deleting is:

$$
\begin{bmatrix}
J_{l_1} & & & & & \\
& J_{l_2} & & & & \\
& & \ddots & & & \\
& & & J_{l_k}
\end{bmatrix},
$$

(28)

and the counterpart of Eq. (25) by subtraction and deleting is:

$$
\begin{bmatrix}
J_{l_1} & & & & & \\
& J_{l_2} & & & & \\
& & \ddots & & & \\
& & & J_{l_k}
\end{bmatrix},
$$

(29)

where $\bar{J}_{l_k}$ is an $(l_k - 1) \times (l_k - 1)$ matrix of form Eq. (25). To clarify, the last row of the above big matrix is $(1, 1, \ldots, 1, 2)$. It is easy to perform row transformation on the above matrix and get:

$$
\begin{bmatrix}
K_{l_1} & & & & & \\
& K_{l_2} & & & & \\
& & \ddots & & & \\
& & & K_{l_k}
\end{bmatrix},
$$

(30)

where $K_l = \text{diag}\{1, \ldots, 1, 0\}$ (size $l$), $\bar{K}_l = \text{diag}\{1, \ldots, 1, l\}$ (size $l - 1$). To clarify, the last row of the above big matrix is $(0, \ldots, 0, l_1, 0, \ldots, 0, l_2, \ldots, 0, \ldots, 0, l_k)$. Therefore, the structure of $Q(n, a, b)$ is:

$$
Q(n, a, b) = \mathbb{Z}^{k-1} \oplus \mathbb{Z}_{\gcd(l_1, \ldots, l_k)}
$$

(31)

where $\mathbb{Z}_{\gcd(l_1, \ldots, l_k)}$ is the greatest common divisor and $\mathbb{Z}_1$ means trivial group $\{0\}$ if $\gcd = 1$.

The $\mathbb{Z}^{k-1}$ comes from the fact that we have $k$ groups of bands (bands that transfer to each other under braidings are in the same group). Each band has an integer Chern number, with summation equals 0. This is the same as the Hermitian case. However, there is an extra $\mathbb{Z}_{\gcd}$. We also see that the extra torsion part is determined by all band groups as a whole, not from any specific band group. It shows some complicated interplay between energy braiding and eigenstates topology.

With other permutations $a, b (a, b \neq id)$, it is possible to get more than one torsions. An example is $a : 1 \leftrightarrow 2, 3 \leftrightarrow 4$ with $b : 1 \leftrightarrow 3, 2 \leftrightarrow 4$. The algorithm will give us $\mathbb{Z}_2 \oplus \mathbb{Z}_2$.

## V. Instability

Examples in Sec. IV show that our homotopical approach reveals more topological invariants than traditional $K$-theory approach. For example, a 2-band Chern “insulator” in 2D may reveal some $\mathbb{Z}_2$ classification due to nontrivial topology of the spectrum.

Similar phenomena also happen in the Hermitian world. For example, in three dimensions (3D), insulators
in class A are always trivial according to the periodicity table. However, one can still have a $\mathbb{Z}$ classification if the number of bands is fixed to be 2, due to the fact that $\tau_3(\mathbb{C}P^1) = \mathbb{Z}$. This is called the Hopf insulator [67], which is unstable against adding more bands. Indeed, as long as one adds one more band above and below the Fermi surface respectively, the classification will be trivial due to $\tau_3(Gr_3(3,1)) = 0$ (and similarly for more bands), where $Gr_3(3,1)$ is the complex Grassmannian.

A natural question arises: is our new topological invariants stable against adding bands?

As an example, let us consider 2-band systems in 2D as in Sec. IV B, and add one more band. Since the classification is decomposed into braiding sectors and each sector has its own classification set, it only makes sense to add a band with no permutation to previous bands (therefore it does not alter the braiding sectors). For each sector $(a,b)$, adding a band without permutation is to add a length-1 cycle after previous $a,b$.

- $a, b$ even. Then $a'$ and $b'$ are trivial permutations, therefore $Q(3,a,b) = \mathbb{Z}^2$, which are just two Chern numbers.

- $a$ even, $b$ odd. Then $a'$ trivial while $b'$ decomposes as $(12)(3)$. Eq. (31) shows that $Q(3,a',b') = \mathbb{Z}$.

- $a$ odd, $b$ even. Same as above.

- $a, b$ odd. Then both $a'$ and $b'$ has the form $(12)(3)$. A Smith normal form calculation shows $Q(3,a',b') = \mathbb{Z}$.

In all cases, we see that the extra band contributes a Chern number $\mathbb{Z}$, as well as kills the old $\mathbb{Z}_2$ invariant it there is any, even if the $\mathbb{Z}_2$ comes from other bands that never intersect with the added band. This is possible since the $\mathbb{Z}_2$ not just comes from those two bands, but from all three bands as a whole, as noted at the end of Sec. IV C.

The instability of $\mathbb{Z}_2$ can be understood as follows. Assuming $a$ odd and $b$ even, consider the procedure shown in Fig. 3: we start with three bands with Chern number 1, $-1, 0$ respectively, where the first two bands switch to each other after $2\pi$ as in Fig. 2(a). Adding a negative bump and a positive bump in band 1, as well as a positive bump and a negative bump in band 3; then move the rightmost bump pair in band 1 and 3, so that the positive bump cancels the negative bump in band 2; the remaining bumps in band 1 and 3 can be easily canceled, leaving three trivial bands. During the procedure, the local neutral condition is always satisfied. Note that it is essential to have the 3rd band for this to work.

Similarly, as long as $b = id$, Eq. (31) shows that $Q(n + 1, a', b')$ has no torsion part.

We can prove a general result regarding the instability, even if $b \neq id$. For a system with $n$ bands, consider the braiding sector labeled by the commuting pair $(a,b)$. Let us add an extra no-permutation band, denote $a, b \to a', b'$.

The matrix of auxiliary “generators” is:

$$
\begin{bmatrix}
A & B \\
0 & 0
\end{bmatrix}
$$

where $A$ and $B$ are of form Eq. (28) up to some congruent transformation by permutation matrices. The matrix of generators (counterpart of Eq. (25)) is therefore just

$$
[ A \mid B ]
$$

We claim that the invariant factors in its Smith normal form must be 1. Indeed, we claim a more general statement:

**Claim.** Assuming a matrix has the following property: there are either 2 or 0 nonzero elements in each column; in the former case, there is exactly one 1 and one -1. Then the invariant factors of this matrix must be 1 (if there is any).

**Proof.** We prove by induction on the total number of nonzero elements $N$. From the assumption, $N$ must be even. If $N = 0$, then the statement is trivially true.

Now assume the state is true for $N$ and less, let us consider $N + 2$. Denote the matrix to be $A$. Without lose of generality, assume $A_{1,1} = 1$, $A_{2,1} = -1$, $A_{1,1} = 0$ for $i \geq 3$. Add row 1 to row 2, denote the new matrix as $A'$, then $A'_{i,1} = 0$ for $i \geq 2$. Moreover, from the assumption on matrix $A$, there are only 7 possibilities happened to

$$
\begin{bmatrix}
A_{1,2} \\
A_{2,2}
\end{bmatrix}
$$

we only write 4 of them, the other 3 are obtained
by adding negative sign):

\[
\begin{pmatrix}
0 \\
0
\end{pmatrix} \rightarrow \begin{pmatrix}
0 \\
0
\end{pmatrix}, \begin{pmatrix}
1 \\
-1
\end{pmatrix} \rightarrow \begin{pmatrix}
1 \\
1
\end{pmatrix}, \begin{pmatrix}
1 \\
1
\end{pmatrix} \rightarrow \begin{pmatrix}
1 \\
1
\end{pmatrix}.
\]

Therefore, the column \((A_{2,1}', \cdots, A_{n,2}')^T\) satisfies the same assumption as columns of \(A\). The number of nonzero elements in this shorter column is less or equal to that in \((A_{1,2}, \cdots, A_{n,2})^T\). Other columns are similar.

Then we use column transformations to make \(A'_{1,i} = 0\) for \(i \geq 2\), while keeping other elements. \(A'\) is of the form:

\[
A' = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & A''
\end{bmatrix}.
\]

We can then apply the induction assumption on \(A''\) and finish the proof.

Therefore, \(Q(n+1, a', b')\) is always of the form \(\mathbb{Z}^k\). This means all torsion invariants \(\mathbb{Z}_i (i \geq 2)\) are unstable against adding a no-permutation band.

VI. CONCLUSION AND OUTLOOK

In this article, we considered the homotopical classification of non-Hermitian band structures from first principles. We found that, the whole classification set is decomposed into several sectors, based on the braiding of energy levels. Fix a braiding pattern, we consider the classification coming from nontrivial eigenstates topology. Due to the fact that different bands will transfer to each other under braidings, the classification of band topology is not just a direct summation of Chern numbers. Instead, the interplay between energy level braiding and eigenstates topology gives some new torsion invariants.

The torsion invariants come from all bands as a whole, instead of some specific band group. Namely, even if we add a band with no crossing with previous bands, the torsion invariants can in principle be changed. We found that the torsion invariants are unstable, in the sense that just adding a trivial band can trivialize them. This statement is proved based on an interesting combinatorial argument.

There are definitely many works that can be done in this framework. First of all, due to the complexity of the braiding group, it is complicated to describe its conjugacy classes and commuting pairs, let alone the conjugacy classes of commuting pairs. It will be useful to develop more explicit descriptions of the braiding sectors. On the other hand, in this paper we only consider the case with no symmetry as an illustration. It is interesting to consider other symmetry classes using our framework.

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Appendix A: Some algebraic topology details

1. Homotopy class \( \langle T^2, X \rangle \)--proof of Eq. (15)

In this section, we prove Eq. (15) in detail:

\[
\langle T^2, X \rangle \equiv \{(a, b) \in \pi_1(X)^2|ab = ba\} \times \pi_2(X)/(t - t^a, t - t^b | t \in \pi_2). \tag{A1}
\]

Namely, a homotopy class \([f] \in \langle T^2, X \rangle\) one-to-one corresponds to an element in set at right hand side of Eq. (A1).

For each pair \((a, b) \in \pi_1(X)^2\) such that \(ab = ba\), we choose and fix two loops\(^4\) \(a_0, b_0\), and also choose and fix a homotopy from \(a_0b_0^{-1}b_0^{-1}\) to 0, denoted by \(F(a, b)\). Note that \(a_0, b_0, F(a, b)\) are arbitrarily chosen. But once they are chosen, they are fixed for all.

Given \([f] \in \langle T^2, X \rangle\), we choose a map \(f : T^2 \to X\) in this class. There are two nontrivial loops (fixed) in \(T^2\), denoted by \(l_1, l_2\), with the same base point. The restriction of \(f\) on \(l_1\) defines a map (loop) \(f_1 : S^1 \to X\) and therefore an element \(a \in \pi_1(X)\). Similarly we have \(b \in \pi_1(X)\). Since the loop \(l_1l_2^{-1}l_2^{-1}\) is homotopic to 0 in \(T^2\), we know \(ab = ba\) in \(\pi_1(X)\). Obviously \(a, b\) are well-defined function of \([f]\).

Since loop \(f_1\) is homotopic to \(a_0\), there exists (not unique) a homotopy \(F(a)\) from \(f_1\) to \(a_0\); the same for \(b\) and we have a \(F(b)\). Now define an element \(h\) in \(\pi_2(X)\) as in Fig. 4(a). In this way we get an element \(\tilde{h} \in \pi_2(X)/(t - t^a, t - t^b | t \in \pi_2)\).

We need to prove that \(h\) does not depend on the choice of \(f, F(a), F(b)\). To do this, assume we choose a different \(f'\) and therefore different loops \(l_1', l_2'\) in \(X\), different homotopy \(F'(a)\) and \(F'(b)\), and different element \(h' \in \pi_2(X)\). To compare \(h\) and \(h'\) we need to fix a base point. Defined \(t\) to be the element in \(\pi_2(X)\) determined by \(F(a), F'(a)\) and the homotopy between \(f, f'\), see Fig. 4(b). Also from this figure, we know that

\[
h' = h + t - t^b + s - s^a, \tag{A2}
\]

therefore \(\tilde{h} = \tilde{h}'\).

The inverse map is easy to define. Therefore we have proved Eq. (A1).

\(^4\) Note the notations here: \(a, b\) are homotopy class of loops, \(a_0, b_0\) are loops.
FIG. 5. An illustration for the proof of Eq. (17). Assuming $\gamma$ action takes an element in $\pi_2(F_n/S_n)$ (represented by $A$) to $B$, then the lift $\tilde{f}_1$ will be a homotopy from $A$ to $B$. To identify the corresponding element of $\tilde{B}$ in $\pi_2(F_n/S_n)$, just consider $g^{-1}(\tilde{B})$ since it is the same as $\tilde{B}$ under projection.

$\tilde{f}_1(s_0) = \tilde{\gamma}(1), \tilde{f}_0(s_0) = \tilde{\gamma}(0)$. In order to identify the corresponding element of $\tilde{f}_1$ in $\pi_2(F_n/S_n)$, one just need to consider $g^{-1} \circ \tilde{f}_1$ since they $(g^{-1} \circ \tilde{f}_1)$ and $(\tilde{f}_1)$ are the same map after projection to $F_n/S_n$ and $g^{-1} \tilde{f}_1(s_0) = \tilde{f}_0(s_0)$ is the correct base point, see Fig. 5 for illustration of above argument.

Now we identify $g^{-1} \circ \tilde{f}_1$ in $\pi_2(F_n) = \mathbb{Z}^{n-1}$ according to the injection $\pi_2(F_n) \xrightarrow{\partial} \pi_1(C^n)$ in Eq. (8). Recall that the boundary map $\partial$ is defined by a homotopy lifting. For example, to identify $\partial(\tilde{f}_1)$, one regard $\tilde{f}_0 : S^2 \to F_n$ as a map $I^2 \to F_n$, where $\tilde{f}_0(\partial I^2) = \{b_0\}$; then as a homotopy $H_t : I^1 \to F_n$. Then lift $H_0$ along into $GL(n)$. This is just the trivial map to a point, say $e_0$. They use relative homotopy lifting property to lift $H_t$ for $t \in I$. $H_t(I)$, which is the lift of $\tilde{f}_0$ on $I \times \{1\}$, is now a loop based on $e_0$, which induces as an element in $\pi_1(C^n)$.

In our case, $g^{-1} \circ \tilde{f}_1$ is just given by Fig. 6(a). We can construct the lifting explicitly. First note that $S_n$ has an action on $GL(n)$ by column transformation, which is the lift of its action on $F_n$. We lift the path $g^{-1}(\tilde{\gamma})$ in $F_n$ to a path $\beta$ in $GL(n)$ starting at $e_0$. We can make it end at $e_{-1} = g^{-1}e_0$ by gradually changing the phases of each column vector along the path. Now the homotopy lifting is defined as follows (see Fig. 6(b)). For $t \in [0, 1]$, scan the square in Fig. 6(a) from bottom to up. For small $t$ (before touching the inner square), just lift the homotopy it along $\beta$. Then one lifts the homotopy inside the inner square by $g^{-1} \circ$ the homotopy lifting of $\tilde{f}_0$. After one passes the inner square, one can just move $e_{-1}$ to $e_0$ by shrinking the line $\beta$. The homotopy class ($n$ integers) of the loops on fibers is invariant (For example, since we are only looking at the bundle over an open path $\tilde{\gamma}$, we can regard it as a trivial bundle). The final lifting is a loop on the fiber over $b_0$ with base point $e_0$. It is easy to see this loop corresponds to (17).