

Beyond characteristic equations: A unified one-dimensional non-Bloch band theory via wavefunction data

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Non-Hermitian systems play a central role in nonequilibrium physics, where determining the energy spectrum under open boundary conditions is a fundamental problem. Non-Bloch band theory, based on the characteristic equation $\det[E - H(\beta)] = 0$, has emerged as a key tool for this task. However, we show that this framework becomes insufficient in systems with certain symmetries, where identical characteristic equations can yield different spectra. To resolve this, we develop a unified theory that incorporates additional wavefunction information beyond the characteristic equation. Our framework accurately captures spectral properties such as the energy spectrum and the end-to-end signal response in a broad class of systems, particularly those with high symmetry. It reveals the essential role of wavefunction information and symmetry in shaping non-Hermitian band theory.

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Introduction. In recent years, there has been a remarkable surge in research interest surrounding non-Hermitian systems. Such systems naturally arise in open quantum systems [1–5] and in photonic setups with gain and loss [6–16]. The distinctive spectral characteristics of non-Hermitian systems, particularly the emergence of exceptional points, have been recognized as playing a central role in a wide range of applications, including lasing and coherent perfect absorption [17–21]. Among various non-Hermitian phenomena, the non-Hermitian skin effect (NHSE) [22–28] has attracted particular attention due to its profound implications for fundamental physical principles. In particular, the NHSE leads to a striking breakdown of conventional Bloch band theory and a collapse of the bulk-boundary correspondence, thereby challenging the foundational understanding of band structures in Hermitian systems.

The breakdown of conventional Bloch band theory in predicting open-boundary energy spectra poses a fundamental challenge in non-Hermitian system studies, demanding innovative approaches to compute the energy spectra. The theory that addresses this issue is referred to as non-Bloch band theory [22,29–31]. The main idea can be summarized as follows: replace the conventional Bloch wave vector through the substitution $e^{ik} \rightarrow \beta$, thereby mapping the original non-Hermitian Bloch Hamiltonian $H(k)$ to its non-Bloch counterpart $H(\beta)$. The spectral determination process hinges on solving the characteristic equation $\det[E - H(\beta)] = 0$. By solving the zeros of this equation with respect to β and applying the condition to get the continuum

bands, one can trace out a complex manifold of β values, which is referred to as the generalized Brillouin zone (GBZ) [22,23,29,32–40]. This complex-plane trajectory fundamentally serves as the spectral determinant that replaces conventional Brillouin zone concepts. For convenience, we call the condition to get the continuum bands the GBZ condition. The above description tells that the input information of the non-Bloch theory is the characteristic function $\det[E - H(\beta)]$, and once this is determined, the energy spectrum “seemingly” can be obtained through a standard procedure.

Although the GBZ condition derived in non-Bloch band theory successfully applies to many systems [29], it has been shown to fail in certain cases where specific symmetries are present [35,41–43]. A common remedy is to modify the GBZ condition in a manner tailored to the corresponding symmetry. However, we find this approach largely *ad hoc* and lacking in generality, which we regard as unsatisfactory. In parallel, other studies have explored this issue in more general contexts based on the algebraic structure of the characteristic function $\det[E - H(\beta)]$ [32,44]. These works suggest that changes in the GBZ condition can be systematically understood through this algebraic structure. In our recent investigation, we present a counterexample that challenges this interpretation: We identify systems that share the same non-Bloch characteristic equation, yet exhibit distinct energy spectra and GBZs. This finding indicates that the characteristic equation alone is insufficient to fully determine the energy spectrum in certain cases, pointing to a fundamental limitation of the current non-Bloch band theory.

This naturally raises the question: What additional information is required, beyond the characteristic function $\det[E - H(\beta)]$, to fully determine the energy spectrum under open boundary conditions? The answer actually lies in the wavefunction data. Here, the wavefunction data mean the following: The roots β of the characteristic equation, often referred to as generalized eigenvalues, extend the notion of

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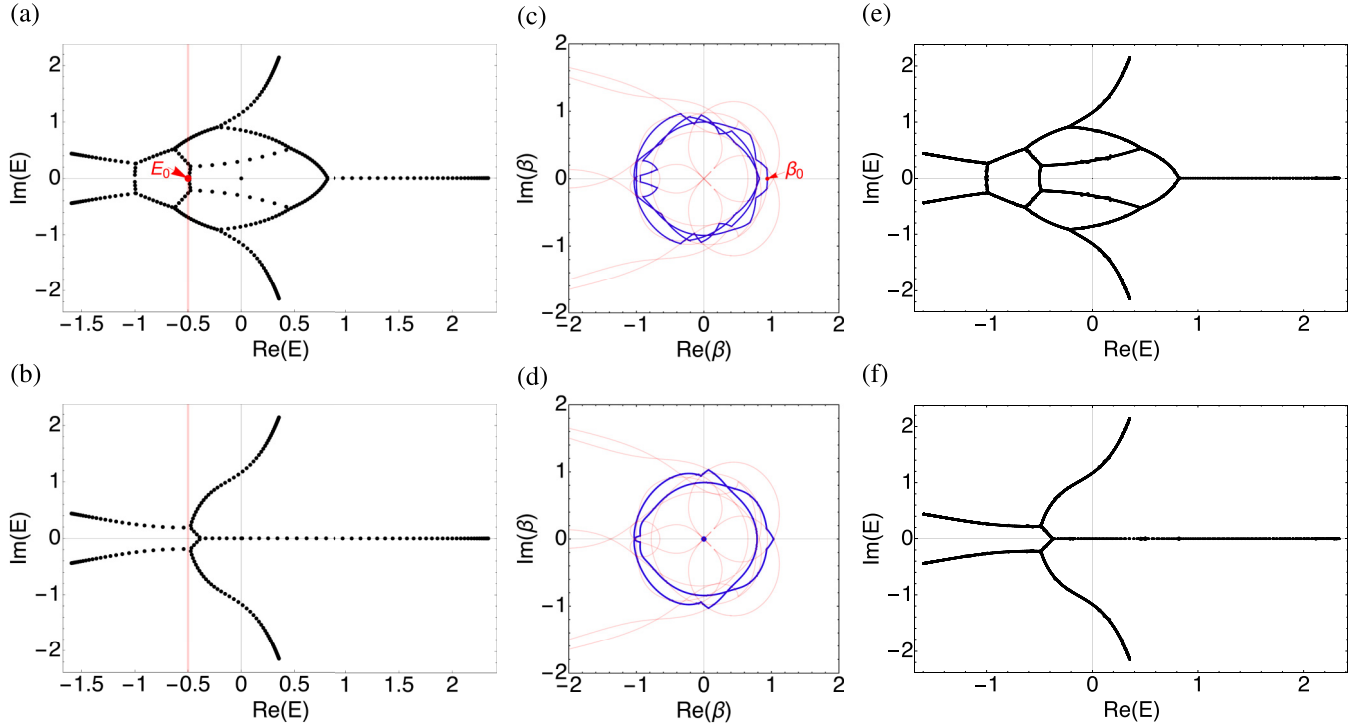


FIG. 1. The open boundary spectra and GBZs of two models, $H_1(k)$ and $H_2(k)$, which share the same characteristic function. The parameters are set as $t_0 = 1$ (energy unit) and $a = b = c = d = 1$ (dimensionless). Panels (a), (c), and (e) correspond to properties of H_1 , while panels (b), (d), and (f) correspond to those of H_2 . (a), (b) Numerically computed spectra for a finite chain of length $L = 100$. The energy $E_0 = -1/2$ lies within the spectrum of H_1 but not within that of H_2 . Faint red vertical lines represent $\text{Re}(E) = -1/2$ in both panels. (c), (d) The GBZs of two models, shown as blue curves. Both models share the same auxiliary GBZ, plotted as faint red curves for reference. Notably, the GBZ in panel (d) includes $\beta = 0$. In the GBZ of H_1 , the mode with generalized momentum β_0 corresponds to the energy E_0 , whereas β_0 does not lie on the GBZ of H_2 . (e), (f) Spectra reconstructed from the GBZs (c) and (d), respectively, representing the open boundary spectra in the limit $L \rightarrow \infty$.

eigenvalues in linear algebra and encode the spatial decay or growth of the wavefunction. Correspondingly, one can define generalized eigenvectors $v(\beta)$ that satisfy $[E - H(\beta)]v(\beta) = 0$, capturing the internal structure of the wavefunction within a unit cell. We find that the pair $(\beta, v(\beta))$ provides a complete description of the energy spectrum. Within this framework, we achieve a unified formulation of non-Bloch band theory that applies to systems with arbitrary symmetries. Moreover, this approach allows for the straightforward algebraic computation of quantities such as the end-to-end signal amplification factor [45–49], which is often difficult to evaluate in systems with high symmetry. For example, in non-Hermitian systems belonging to the symplectic class, the formula for the end-to-end signal amplification factor given in Refs. [45,46] does not hold. To the best of our knowledge, no analogous formula applicable to such systems has been reported in the literature, and in this work we provide the corresponding expression.

Missing information in characteristic function. Previous studies have all taken the characteristic function as their starting point, whereas our work is motivated by a counterexample demonstrating that using the characteristic function alone as the input of the theory is fundamentally incomplete. Figure 1 shows two triple-band non-Hermitian Hamiltonians with the same characteristic function. Figure 1(a) is the open boundary spectrum of

the Bloch Hamiltonian $H_1(k) = \begin{pmatrix} t_0 e^{ik} & b t_0 & 0 \\ a t_0 e^{ik} & t_0 e^{ik} & d t_0 e^{-ik} \\ 0 & c t_0 e^{-ik} & t_0 e^{ik} \end{pmatrix}$ and Fig. 1(b) is the open boundary spectrum of the Bloch Hamiltonian $H_2(k) = \begin{pmatrix} t_0 e^{ik} & 0 & 0 \\ 0 & t_0 e^{ik} & t_0 (a b e^{2ik} + c d e^{-ik}) \\ 0 & t_0 e^{-ik} & t_0 e^{ik} \end{pmatrix}$.

By performing a variable substitution $e^{ik} \rightarrow \beta$, both models result in the same characteristic function $\det[E - H_i(\beta)] = (E - t_0 \beta)(t_0^2 \beta^2 - 2 t_0 E \beta - a b t_0^2 \beta + E^2 - \frac{c d t_0^2}{\beta^2})$, $i = 1, 2$. However, the energy spectra of the two not only are different but also cannot be contained within each other. This difference highlights a fundamental limitation of non-Bloch band theory when the characteristic function is taken as the sole input: The theory is incomplete. One may observe that H_2 is a decoupled Hamiltonian, which causes its GBZ condition to differ from the conventional form. While this observation is correct, a more accurate interpretation is that the symmetry of H_2 enforces a modification of the GBZ condition. Indeed, it is not only decoupling but also other types of symmetry, such as the symplectic symmetry, that can alter the GBZ condition.

To explain the spectrum difference between these two models, we need a new theory with other input data beyond the characteristic function that captures the difference of $H_1(k)$ and $H_2(k)$. Before introducing our modified non-Bloch band theory, we first provide a brief review of the conventional

formulation and highlight key aspects that are typically overlooked in its derivation.

Review of non-Bloch band theory. Start from a one-dimensional tight-binding model in an open chain. Assume its Bloch Hamiltonian is given by $H(k) = \sum_{n=-m}^m a_n e^{ikn}$, with $a_{-m}, a_{-m+1}, \dots, a_m$ being $2m+1$ hopping matrices with dimension l , and the corresponding tight-binding Hamiltonian is $H = \sum_l \sum_{n=-m}^m a_n c_{l+n}^\dagger c_l$. The ansatz for the wavefunction is assumed to be $\psi(n) = \beta^{-n} \psi(0)$, where $\psi(n)$ represents the wavefunction amplitude at the n th unit cell and β represents the spatial decay rate. Due to the translation symmetry in the bulk, the bulk equation is a characteristic equation

$$\det[E - H(\beta)] = 0, \quad (1)$$

where $H(\beta)$ is a reformulation of $H(k)$ by performing a variable substitution $e^{ik} \rightarrow \beta$. This is an algebraic equation of both β and E . For each E , there are $2M$ ($M = ml$) roots of β by taking into account the zero root and the root at infinity, which can be sorted by their magnitudes: $|\beta_1(E)| \leq |\beta_2(E)| \leq \dots \leq |\beta_{2M}(E)|$. The boundary condition gives extra equations, which involve the following [29]:

$$\sum_P F_P \prod_{k \in P} (\beta_k)^L = 0, \quad (2)$$

where the set P is a subset of the mode index set $\{1, 2, \dots, 2M\}$ with M elements, F_P is a scalar for each P , and L is the length of the one-dimensional chain. To produce the continuum band, the magnitude of the leading-order term and the next-to-leading-order term of Eq. (2) must be equal. This requirement leads to the condition $|\beta_{2M}\beta_{2M-1} \dots \beta_{M+2}\beta_{M+1}| = |\beta_{2M}\beta_{2M-1} \dots \beta_{M+2}\beta_M|$, which is equivalent to $|\beta_M| = |\beta_{M+1}|$ [29]. This condition is known as the GBZ condition, as it determines the shape of the GBZ.

However, the above derivation overlooks an important subtlety: It does not account for the possibility that the coefficients F_P of terms $\beta_{2M}\beta_{2M-1} \dots \beta_{M+2}\beta_{M+1}$ and $\beta_{2M}\beta_{2M-1} \dots \beta_{M+2}\beta_M$ in Eq. (2) may vanish, i.e., $F_{M+1, M+2, \dots, 2M} = 0$ or $F_{M, M+2, \dots, 2M} = 0$. In such cases, these terms no longer represent the true leading-order contributions, and consequently, the standard GBZ condition $|\beta_M| = |\beta_{M+1}|$ no longer applies.

As we have shown in Fig. 1, changes in the GBZ condition of this kind cannot be inferred from the characteristic function $\det[E - H(\beta)]$. In other words, the vanishing of the coefficients F_P is not encoded in the characteristic function, and the central contribution of this work is a criterion for determining when $F_P = 0$ by using the extra information beyond the characteristic function, which will be introduced in the following.

Wavefunctions and the completeness criterion. In Eq. (1), we discuss the characteristic equation whose solutions β_i ($i = 1, \dots, 2M$) physically represent the spatial decay or growth rates of the eigenmodes. For each mode i , the wavefunction inside the unit cell satisfies

$$[E - H(\beta_i)]v_i = 0. \quad (3)$$

In other words, the wavefunction ansatz of the mode i is $\psi(n) = \beta_i^{-n} v_i$. It is quite easy to solve v_i since $[E - H(\beta_i)]$ is a matrix with dimension l , which is a small size. For convenience, we call β_i the generalized eigenvalues of the characteristic equation and v_i the generalized eigenvector of

the generalized eigenvalue β_i . Similarly, there are also left generalized eigenvectors u_i that satisfy

$$u_i^T [E - H(\beta_i)] = 0. \quad (4)$$

Left and right generalized eigenvectors all encode the wavefunction information. In the following, we explain how to express the GBZ condition in terms of this wavefunction information. First, note that $M = ml$, where l is the dimension of Hamiltonian $H(\beta)$. We can construct supercell right generalized eigenvectors

$$x_i = \begin{pmatrix} v_i \\ \frac{1}{\beta_i} v_i \\ \vdots \\ \left(\frac{1}{\beta_i}\right)^{m-1} v_i \end{pmatrix} \quad (5)$$

and supercell left generalized eigenvectors

$$y_i = \begin{pmatrix} u_i \\ \beta_i u_i \\ \vdots \\ \beta_i^{m-1} u_i \end{pmatrix}. \quad (6)$$

It can be seen that they are corresponding wavefunctions inside the supercell with m unit cells, which is quite easy to calculate since $m = M/l$ is quite small. The above form relies on the assumption that all β_i are nondegenerate, and the form of the degenerate case can be seen in the Supplemental Material [50], which is inspired by Ref. [51] and derived independently in Refs. [52,53]. Now we can express the criterion for determining when $F_P = 0$ in Eq. (2), i.e.,

$$F_P \neq 0 \iff \det\left(\sum_{i \in P} x_i y_i^T\right) \neq 0. \quad (7)$$

There are M terms in $\sum_{i \in P} x_i y_i^T$ and each term $x_i y_i^T$ is a $M \times M$ matrix of rank 1. Hence, Eq. (7) can be understood as a biorthogonal completeness relation; it tells whether or not these M modes from the subset P can span the whole Hilbert space. Our additional GBZ condition states that for the term $\prod_{i \in P} (\beta_i)^L$ to be the leading term of Eq. (2), the corresponding modes from index set P must form a complete basis, which is expressed by the mathematical equation $\det(\sum_{i \in P} x_i y_i^T) \neq 0$. In other words, the leading term of Eq. (2) is the one for which $\det(\sum_{i \in P} x_i y_i^T) \neq 0$ and the product $\prod_{k \in P} |\beta_k|$ is maximized, which can be mathematically expressed as

$$P_{\max} = \arg \max_{P \in \{i_1, \dots, i_M | \det(\sum_{j=1}^M x_{i_j} y_{i_j}^T) \neq 0\}} \prod_{i \in P} |\beta_i|, \quad (8)$$

where $P_{\max}$ denotes the set of mode indices for the leading term, while “arg max” represents the standard mathematical operator for identifying indices of maximal elements—a notation widely used in optimization, mathematics, and computer science. From Eq. (8), it can be seen that Eq. (7) is the key result of this paper, and we put the mathematical derivation in the Supplemental Material [50].

Based on Eq. (8), the algorithm of the modified non-Bloch band theory can be summarized as Fig. 2(b) and can be compared to the original non-Bloch band theory shown in Fig. 2(a).

TABLE I. Biorthogonal completeness of three modes of H_1 at energy $E = -1/2$. The index sets P of the leading-order term and the next-to-leading-order term are indicated in bold. The energy $E = -1/2$ lies within the spectrum since the magnitudes of the leading-order term and the next-to-leading-order term are equal.

P	{4,5,6}	{3,5,6}	{3,4,5}	{3,4,6}	{2,5,6}	{2,4,6}
$\prod_{i \in P} \beta_i $	1.06	1.06	0.94	0.94	0.57	0.5
$\text{rank}(\sum_{i \in P} x_i y_i^T)$	3	3	3	3	3	3
$\det(\sum_{i \in P} x_i y_i^T)$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$

The above theoretical framework may seem abstract; we now validate it using the previously discussed triple-band models, as shown in Fig. 1. In Fig. 1(a), we demonstrate that a specific energy level, $E_0 = -1/2$, lies within the spectrum of H_1 , whereas Fig. 1(b) shows that it does not belong to

the spectrum of H_2 . This discrepancy can be explained using the completeness condition in Eq. (7). By substituting $E = -1/2$ into the characteristic equation [Eq. (1)], we obtain six roots: $\beta_1 = 0$, $\beta_2 = -0.5$, $\beta_3 = -0.94$, $\beta_4 = 0.94$, $\beta_5 = -1.06i$, and $\beta_6 = 1.06i$, ordered by their magnitudes. For each three-element subset P of the index set $\{1, 2, \dots, 6\}$, we test the criterion in Eq. (7). In Tables I and II, we list several such index subsets P that yield large values of $\prod_{i \in P} |\beta_i|$, corresponding to Hamiltonians H_1 and H_2 , respectively. According to Eq. (8), the leading-order term and the next-to-leading-order term are indicated in bold. From Table I, it can be seen that $\beta_4 \beta_5 \beta_6$ and $\beta_3 \beta_5 \beta_6$ serve as the leading-order term and next-to-leading-order term, and the GBZ condition $|\beta_4 \beta_5 \beta_6| = |\beta_3 \beta_5 \beta_6|$ is satisfied. This indicates that $E = -1/2$ lies in the spectrum of H_1 . In contrast, Table II shows that for H_2 , the leading-order term and next-to-leading-order term are given by $\beta_2 \beta_5 \beta_6$ and $\beta_2 \beta_4 \beta_6$, respectively. However, the GBZ condition $|\beta_2 \beta_5 \beta_6| = |\beta_2 \beta_4 \beta_6|$ is not satisfied, which implies that $E = -1/2$ is not part of the spectrum of H_2 . Therefore, Eq. (7) is crucial to determine the GBZ condition and further the GBZ. Based on this criterion, we compute and plot the GBZs for H_1 and H_2 in Figs. 1(c) and 1(d), respectively. The spectra made from these two GBZs that represent the open boundary spectra at the chain length limit $L \rightarrow \infty$ are shown in Figs. 1(e) and 1(f). The above discussion shows that the triples (β_i, v_i, u_i) can be regarded as the input data of our modified non-Bloch theory. In mathematical literature, this terminology already exists: The triple (β_i, v_i, u_i) is referred to as a *Jordan triple*, and the pair (β_i, v_i) as a *Jordan pair* [51].

Application in end-to-end signal response. Above we have discussed the importance of the wavefunction information in determining the energy spectrum. We now turn to discuss its role in computing the physical response, i.e., the Green's function. The non-Hermitian Green's function has numerous applications in physics. For instance, it captures the end-to-end response of field coherence in bosonic open systems [45]. Even in Hermitian mesoscopic transport problems, it serves as an effective mathematical tool that enables convenient computation of nonreciprocal transport [54,55]. These problems

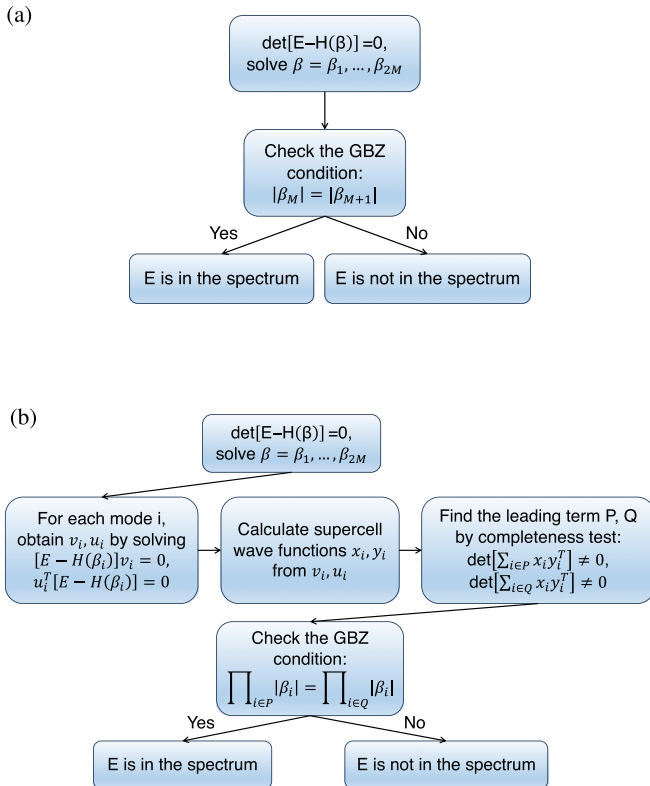


FIG. 2. (a) Workflow of the original non-Bloch band theory algorithm. Only the most common scenario is shown; in systems with symmetry, the GBZ condition may require case-specific treatment. (b) Workflow of the modified non-Bloch band theory algorithm. The application of this algorithm to specific models H_1 and H_2 is illustrated in Tables I and II.

TABLE II. Biorthogonal completeness of three modes of H_2 at energy $E = -1/2$. The index sets P of the leading-order term and the next-to-leading-order term are indicated in bold. The energy $E = -1/2$ is not part of the spectrum since the magnitudes of the leading-order term and the next-to-leading-order term are not equal.

P	{4,5,6}	{3,5,6}	{3,4,5}	{3,4,6}	{2,5,6}	{2,4,6}
$\prod_{i \in P} \beta_i $	1.06	1.06	0.94	0.94	0.57	0.5
$\text{rank}(\sum_{i \in P} x_i y_i^T)$	2	2	2	2	3	3
$\det(\sum_{i \in P} x_i y_i^T)$	$= 0$	$= 0$	$= 0$	$= 0$	$\neq 0$	$\neq 0$

pertain to the end-to-end response of the system. It is known that in general non-Hermitian systems, a signal injected at one end of a chain can be amplified at the other end [56]. This amplification follows an exponential law, described by the Green's function as $\|G_{1L}(\omega)\| = \alpha_{\leftarrow}^L$, where L denotes the chain length, $G_{1L}(\omega) = (\omega - H)_{1L}^{-1}$ is the Green's function from the right end to the left end, and $\|\cdot\|$ represents the absolute value in single-band systems and the matrix norm in multiband systems. The exponential factor $\alpha_{\leftarrow}$ is actually $|\beta_M(\omega)|$ (with respect to the convention adopted here) in a general single-band non-Hermitian systems [45,46]. Here, $|\beta_i(\omega)|$ are solutions of $\det[\omega - H(\beta)] = 0$ and $|\beta_1(\omega)| \leq |\beta_2(\omega)| \leq \dots \leq |\beta_{2M}(\omega)|$. Thus, if $|\beta_M(\omega)| > 1$, the signal is amplified from right to left. Although single-band systems are well understood, a corresponding result for general multiband systems remains lacking. For example, for a Hamiltonian belonging to the symplectic class, should $\alpha_{\leftarrow}$ be given by $|\beta_M(\omega)|$ or $|\beta_{M+1}(\omega)|$? To address this question, we investigate the multiband non-Hermitian Green's function and derive a universal expression for $\alpha_{\leftarrow}$. The first step is to identify the leading contribution that satisfies the completeness relation in Eq. (7); specifically, one must determine an index subset $P_{\min}$ containing M modes that fulfills

$$P_{\min} = \arg \min_{P \in \{i_1, \dots, i_M | \det(\sum_{j=1}^M x_{ij} y_{ij}^T) \neq 0\}} \prod_{i \in P} |\beta_i|. \quad (9)$$

Similar to Eq. (8), Eq. (9) means that $P_{\min}$ represents the term with nonzero $\det(\sum_{i \in P} x_{ij} y_{ij}^T)$ and the smallest $\prod_{k \in P} |\beta_k|$. Then, $\alpha_{\leftarrow}$ can be expressed as

$$\alpha_{\leftarrow} = \max_{i \in P_{\min}} |\beta_i|. \quad (10)$$

This result admits a straightforward interpretation: The Green's function $G_{1L}(\omega)$ receives contributions from the modes in the index set $P_{\min}$ and can be written as $G_{1L}(\omega) = \sum_{i \in P_{\min}} \beta_i^L G_i(\omega)$. Therefore, in the large L limit, the matrix norm $\|G_{1L}(\omega)\|$ is dominated by the exponential growth associated with the largest β_i among these modes, i.e., $\alpha_{\leftarrow} = \max_{i \in P_{\min}} |\beta_i|$.

We test this conclusion using a non-Hermitian Hamiltonian belonging to the symplectic class. The Bloch Hamiltonian is given by $H(k) = \begin{pmatrix} 0 & D_1(k) \\ D_2(k) & 0 \end{pmatrix}$, where $D_1(k) = t \sin k \sigma_x + (\Delta + u + u \cos k + i \frac{\gamma}{2}) \sigma_y$, $D_2(k) = t \sin k \sigma_x + (\Delta + u + u \cos k) \sigma_y$, and σ_i are Pauli matrices. This system has a symplectic $\text{TRS}^\dagger$ operator $\mathcal{U}_T = -i \sigma_y \otimes \mathbb{I}_{2 \times 2}$, under which the Hamiltonian satisfies $\mathcal{U}_T H(k)^T \mathcal{U}_T^{-1} = H(-k)$. In Fig. 3, we plot the end-to-end exponential factor $\alpha_{\leftarrow}$ and compare it with the solutions of the characteristic equation $\det[\omega - H(\beta)] = 0$. This equation yields eight analytical solutions, which we label using Roman numerals for clarity. Among them, four are shown in Fig. 3(a); the other four consist of two solutions ($\beta_{\text{IV}}, \beta_{\text{VI}}$) that lie above and two ($\beta_{\text{III}}, \beta_{\text{VIII}}$) that lie below those depicted. As shown in Fig. 3(a), there are four crossing points, which are potential transition points of the amplification factor $\alpha_{\leftarrow}$. Based on these crossings, the figure can be divided into four distinct regions, labeled A, B, C, and D. As an illustrative example, we focus on region B. In this region, the completeness relation $\det(\sum_{i \in P} x_{ij} y_{ij}^T)$ vanishes for the index set $P = \{\text{III}, \text{VIII}, \text{I}, \text{V}\}$,

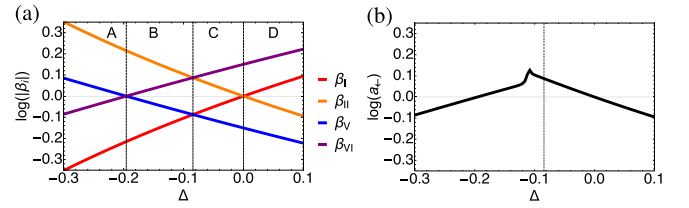


FIG. 3. Comparison between the solutions of the characteristic equation $\det[\omega - H(\beta)] = 0$ and the end-to-end exponential factor $\alpha_{\leftarrow}$. Parameters are set as $t = 1.01$, $u = 1$, $\gamma = 1.2$, and $\omega = 0.01i$. (a) Magnitudes of analytical solutions β_i of the characteristic equation plotted as a function of the parameter Δ . (b) End-to-end exponential factor $\alpha_{\leftarrow}$ as a function of the parameter Δ , obtained via a linear fit of the logarithm of the end-to-end Green's function vs the system length L , with $L \in [150, 170]$.

while it remains nonzero for $P = \{\text{III}, \text{VIII}, \text{I}, \text{VI}\}$. These results are obtained from the structure of the wavefunctions (see the Supplemental Material [50]). Therefore, according to the criterion in Eq. (9), the minimal index set is $P_{\min} = \{\text{III}, \text{VIII}, \text{I}, \text{VI}\}$, and the corresponding spatial exponential factor $\alpha_{\leftarrow} = |\beta_{\text{VI}}|$.

A universal feature is also observed in Fig. 3(b): The spatial exponential factor $\alpha_{\leftarrow}$ exhibits a turning point only at the boundary between regions B and C, while the crossing points at $|\beta| = 1$ (or $\log(|\beta|) = 0$) are not associated with such transitions. This is because the crossing at $|\beta| = 1$ violates the completeness condition due to an exchange of wavefunctions, a result that can be rigorously proven in the Supplemental Material [50]. In summary, according to Eqs. (9) and (10), we find that $\alpha_{\leftarrow} = |\beta_{\text{VI}}|$ in regions A and B, and $\alpha_{\leftarrow} = |\beta_{\text{II}}|$ in regions C and D. This prediction is in excellent agreement with the numerical results shown in Fig. 3(b). However, the question remains: Is $\alpha_{\leftarrow} = |\beta_M(\omega)|$ or $\alpha_{\leftarrow} = |\beta_{M+1}(\omega)|$? Since $|\beta_M(\omega)|$ and $|\beta_{M+1}(\omega)|$ are defined by their magnitudes in ascending order, we can immediately deduce from Fig. 3(a) that $\alpha_{\leftarrow} = |\beta_M(\omega)|$ in regions A and D and $\alpha_{\leftarrow} = |\beta_{M+1}(\omega)|$ in regions B and C. This stands in stark contrast to the single-band case, where $\alpha_{\leftarrow}$ is always equal to $|\beta_M(\omega)|$. In symplectic class systems, $\alpha_{\leftarrow}$ can take either value, and its precise value is determined by Eqs. (9) and (10). Importantly, distinguishing whether $\alpha_{\leftarrow} = |\beta_M(\omega)|$ or $|\beta_{M+1}(\omega)|$ is crucial for predicting signal amplification, because $|\beta_{M+1}(\omega)|$ that is larger than 1 stands for signal amplification while $|\beta_M(\omega)|$ that is smaller than 1 stands for signal decay.

This behavior of the spatial exponential factor $\alpha_{\leftarrow}$ also reveals a deeper connection to the GBZ condition. Specifically, a turning point in $\alpha_{\leftarrow}$ indicates that the resonance frequency ω enters the spectrum. The universal feature we observed, namely, that crossing points at $|\beta| = 1$ do not correspond to turning points, implies that the GBZ condition in the symplectic class cannot take the conventional form $|\beta_M| = |\beta_{M+1}|$. Interestingly, some previous works have proposed an even stronger and more definitive statement that the GBZ condition is given by $|\beta_{M+1}| = |\beta_{M+2}|$. However, we emphasize that the validity of this conclusion is contingent upon a prerequisite: There are no other symmetries that further alter the completeness among the wavefunctions. For example, if the system possesses two distinct symplectic symmetries

$\mathcal{U}_{T,1}$ and $\mathcal{U}_{T,2}$, then the spatial exponential factor $\alpha_{\leftarrow}$ may instead correspond to $|\beta_{M+2}(\omega)|$, and the GBZ condition may accordingly shift away from $|\beta_{M+1}| = |\beta_{M+2}|$. Nevertheless, regardless of how many symmetries the system possesses, our expressions for the spatial exponential factor $\alpha_{\leftarrow}$ in Eqs. (9) and (10) remain universally valid. These formulas provide a symmetry-agnostic method for determining $\alpha_{\leftarrow}$, thereby offering a consistent framework even in the presence of complex symmetry structures.

Discussion and conclusion. The results presented in this work focus on one-dimensional non-Hermitian systems. For systems in higher dimensions, the amoeba formulation has been developed as a nontrivial generalization of one-dimensional non-Bloch band theory [31]. It is worth noting, however, that the amoeba formulation still relies solely on the characteristic equation as input, and the issue of GBZ condition shifting remains unresolved [41]. We believe that certain aspects of our results for one-dimensional systems may still be applicable to higher-dimensional cases. For instance, in a two-dimensional system with Hamiltonian $H(\beta_x, \beta_y)$, where β_x and β_y are the generalized complex momenta, one may fix β_y at a value corresponding to a point on the two-dimensional GBZ (i.e., a minimal point in the amoeba) and apply our theory to the resulting pseudo-one-dimensional system along the x direction. In such cases, we expect that the biorthogonal completeness condition given in Eq. (7) remains a necessary condition. Whether Eq. (7) also serves as a sufficient condition in higher dimensions and how to more effectively treat such systems are important questions that we leave for future study.

The one-dimensional non-Bloch band theory has already been verified in experimental settings [57]. However, the

nonstandard GBZ conditions in highly symmetric non-Hermitian systems have not yet been experimentally demonstrated. Our modified theory not only provides a non-*ad hoc* framework at the theoretical level, but its generality also makes it well suited for systematic experimental validation of GBZ theory in such symmetric non-Hermitian systems. Experimentally, mechanical oscillators [58,59], photonic crystals [6–8], and electrical circuit [60,61] represent promising platforms for such investigations.

In summary, our findings highlight a fundamental limitation of conventional non-Bloch band theory: The characteristic equation of a non-Bloch Hamiltonian alone is insufficient to determine the open boundary spectrum. This realization calls for a significant revision of the theoretical framework, motivating the development of an augmented formulation that systematically incorporates wavefunction information as an essential ingredient in spectral analysis. The resulting generalized theory is broadly applicable across non-Hermitian systems and proves particularly effective in high-symmetry settings, where it bypasses the technical difficulties typically associated with analyzing the GBZ condition and the end-to-end signal response.

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Data availability. The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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