We provide a systematic and self-consistent method to calculate the generalized Brillouin Zone (GBZ) from a Hamiltonian. In general, a $m$-band non-Hermitian Hamiltonian is constituted by $m$ distinct sub-GBZs, each of which is a piecewise analytic closed loop. Based on the concept of resultant, we can show that all the analytic properties of the GBZ can be characterized by an algebraic equation, the solution of which in the complex plane is dubbed as auxiliary GBZ (aGBZ). In general, the GBZ is a subset of aGBZ. On the other hand, the aGBZ is the minimal analytic element containing all the informations of GBZ. We also provide a systematic method to obtain the GBZ from aGBZ.

**Introduction** — Non-Hermitian Hamiltonians [1–49] are known to have anomalous bulk-boundary correspondence [24–31, 50–58], when their open boundary eigenstates have non-Hermitian skin modes [24–31, 59–64]. In this case, the “bulk” properties of the open boundary Hamiltonian can never be characterized by the Bloch Hamiltonian [24, 25, 29, 30]. It has been proposed that many important informations of open boundary Hamiltonian can be encoded from the generalized Brillouin zone (GBZ) [24, 25, 29, 30], including the energy spectra [24, 29, 30], phase boundary [24], skin modes [24, 30, 31, 51, 52], topological “boundary” states [24–31, 50–58], and bulk-boundary correspondence [24, 28–30, 52, 65]. Thus calculating the GBZ and understanding its properties draw extensive attentions in this field recently [9, 10, 17, 18, 24–31, 50–57, 66–72].

We first review the procedure of exactly solution in an one-dimensional (1D) Hamiltonian under the open boundary condition [24, 29, 73]. Consider a general $m$-band 1D Hamiltonian without any symmetry in real space

$$
\hat{H} = \sum_{i,j=1}^{N} \sum_{\mu,\nu=1}^{m} t_{ij}^{\mu\nu} c_{i\mu}^{\dagger} c_{j\nu}, \tag{1}
$$

where $t_{ij}^{\mu\nu} \neq (t_{ji}^{\nu\mu})^*$ and $i,j$ and $\mu,\nu$ label the lattice sites and band indexes respectively. Since the discrete translational symmetry is broken at the ends of the 1D lattice, the eigenstates can no longer be described by a single Bloch wave. Physically, this corresponds to the boundary scattering between different Bloch waves with the same energy. As a result, the linear superposition of the scattered Bloch waves form the eigenstate of the open boundary Hamiltonian if the boundary condition is satisfied [74]. However, the algebraic equation determined by the boundary condition is not easy to be carried out analytically in general.

However, if one focuses on the asymptotic solutions in the thermodynamic limit $N \to \infty$, there exist a different procedure to determine the eigenvalues, which is proposed by Ref [24], and extended by Ref [29, 30] and this paper [74]. The procedure can be described as follows. Firstly, write down the characteristic equation of Eq. 1

$$
f(\beta, E) = \det(\mathcal{H}(\beta) - E\hat{1}) = \sum_{i=-p}^{p} \sum_{j=0}^{m} c_{ij} \beta^j E^i = 0, \tag{2}
$$

where $[\mathcal{H}(\beta)]_{\mu\nu} = \sum_{l=-i}^{i} t_{ij}^{\mu\nu} \beta^l$, $t_{ij}^{\mu\nu} = t_{ij}^{\nu\mu} \delta_{i+j,l}$, and $\beta = \exp(i k)$ labeling the Bloch wave with the complex wave-vector $k$ [24]. Secondly, if $f(\beta, E)$ is an irreducible algebraic polynomial [74], we can solve the characteristic equation for a given $E$, and order the solutions by the absolute value as

$$
|\beta_1(E)| \leq |\beta_2(E)| \leq ... \leq |\beta_{p+s}(E)|. \tag{3}
$$

Finally, if $|\beta_p(E)| = |\beta_{p+1}(E)|$, where $p$ is the order of the pole in Eq. 2, then, $E$ is an eigenvalue of $\hat{H}$ in the thermodynamic limit $N \to \infty$. In the second step, if $f(\beta, E)$ is a reducible algebraic polynomial [74], which can be written as the product of a set of irreducible polynomials $f(\beta, E) = f_1(\beta, E)...f_m(\beta, E)$, then, repeat the above procedure for each $f_i(\beta, E) = 0$, where $i = 1,...,m$.

In the following contents, without of special emphasized, $f(\beta, E)$ is assumed to be irreducible algebraic polynomials. In principle, by trying every $E \in \mathbb{C}$, we can obtain all the GBZ spectra (or continuous band spectra) [29],

$$
E_{GBZ} := \{ E \in \mathbb{C} : |\beta_p(E)| = |\beta_{p+1}(E)| \}, \tag{4}
$$

which corresponds to the bulk spectra in Hermitian case. The corresponding GBZ can be obtained from $E_{GBZ}$ by solving the characteristic equation

$$
\beta_{GBZ} := \{ \beta \in \mathbb{C} : \forall E \in E_{GBZ}, |\beta_p(E)| = |\beta_{p+1}(E)| \}. \tag{5}
$$

For the Hermitian case, since the characteristic equation satisfying $f^*(\beta^*, E) = f(1/\beta, E)$ [74], $\beta_{GBZ}$ is the unit.
circle in the complex plane, which coincides with the conventional Brillouin zone (BZ) defined under the periodic boundary condition. Consequently, the Bloch Hamiltonian \( \mathcal{H}(k) \) faithfully describes the physical properties in Hermitian cases with open boundary condition. However, for the non-Hermitian Hamiltonian, \( \beta_{\text{GBZ}} \) is not restricted to be unit circle in general, which results in the anomalous bulk-boundary correspondence as proposed in Ref [24].

This paper is motivated by the following question: can we express the 1D GBZ as some analytic functions of \((\text{Re } \beta, \text{Im } \beta)\)? The answer to this question is not only of conceptual importance but also of practical significance. On the one hand, a deeper understanding of GBZ requires its analytic properties. On the other hand, the calculation of the GBZ requires the numerical diagonalization of the non-Hermitian Hamiltonian, whose computing time and numerical errors are sensitive to the lattice size [74], thus the results may not be faithful and reliable [74, 75]. In this paper, we show that the GBZ of Eq. 2 has \( m \) distinct sub-GBZs, corresponding to the \( m \) distinct bands. Each sub-GBZ is a piecewise analytic closed loop, and can be described by a common algebraic equation, which is dubbed as auxiliary GBZ (aGBZ) and can be calculated based on the concept of resultant of polynomials [74, 76–78]. It should be emphasized that the aGBZ contains redundant informations which do not belong to the GBZ. We also provide a systematic method to pick up the GBZ from aGBZ.

**Auxiliary GBZ** — As discussed in foregoing section, the GBZ is determined uniquely by the characteristic equation \( f(\beta, E) = 0 \) and its root relation \( |\beta_p(E)| = |\beta_{p+1}(E)| \) for any given \( E \in \mathbb{C} \), where \( p \) is the order of the pole of \( f(\beta, E) = 0 \). Since it is hard to order the roots of Eq. 2, we reasonably relax the root relation to be \( |\beta_j(E)| = |\beta_{j+1}(E)| \) for arbitrary \( j = 1, \ldots, p + s - 1 \). Combining the characteristic equation and the relaxed root relation, one can obtain

\[
f(\beta, E) = f(\beta e^{i\theta}, E) = 0.
\]

Since there exist five variables \((\text{Re } \beta, \text{Im } \beta, \text{Re } E, \text{Im } E, \theta)\) and four constraint equations \( f = \text{Im } f = \text{Re } f^g = \text{Im } f^\theta = 0 \) where \( f^g := f(\beta e^{i\theta}, E) \), the solution of Eq. 6 is 1D curve in the 5D parameter space. Therefore, all the informations of GBZ are contained by the projection of these curves in the complex \( \beta \)-plane. This is the aGBZ and can be expressed formally as follows

\[
F_{\text{aGBZ}}(\beta, \text{Im } \beta) = 0.
\]  

Next we show the method to derive Eq. 7 from Eq. 6 and provide a criterion to determine the GBZ from the aGBZ.

From Eq. 6 to Eq. 7, one just need to eliminate \( E \) and \( \theta \) in the constraint equations. Mathematically, the resultant [74, 76–79] of two polynomials provides a powerful tool in the elimination theory. We first apply the method to eliminate \( E \) from Eq. 6. Starting from \( f = \prod_{\mu=1}^{p+1}[E - E_\mu(\beta)] \), \( f^g = \prod_{\mu=0}^{p}[E - E_\mu(3\delta e^{i\theta})] \), where \( E_{\mu}(\beta) \) is the \( \mu \)-th eigenenergy of the Hamiltonian \( \mathcal{H}(\beta) \), their resultant with respect to \( E \) is defined as \( R^{f,f^g}(\beta, \theta) := \prod_{\mu,\nu=1}^{p+1}[E_\mu(\beta) - E_\nu(\beta e^{i\theta})] \). Now suppose that there exist some \( \beta_0 \) and \( \theta_0 \) satisfying \( E_{\mu}(\beta_0) = E_{\nu}(\beta_0 e^{i\theta_0}) \), their resultant \( R^{f,f^g}(\beta_0, \theta_0) \) must be zero, and \( f = 0 \) and \( f^g = 0 \) must have common root \( E = E_{p}(\beta_0) = E_{\nu}(\beta_0 e^{i\theta_0}) \). It can be proved that \( f = 0 \) and \( f^g = 0 \) have common roots if and only if their resultant \( R^{f,f^g} \) is zero [74]. Although the resultant is defined by the eigenvalues of \( \mathcal{H}(\beta) \), it can be calculated from the Sylvester matrix easily and systematically [74].

Next step is to eliminate \( \theta \) from \( R^{f,f^g}_\theta = R^{f,f^g}_\theta(\beta, \text{Im } \beta) \). Since \( R^{f,f^g}_\theta \) are algebraic polynomials of \( \sin \theta \) and \( \cos \theta \), they can not be directly eliminated by the resultant. The standard way is to use the Weierstrass substitution \( \cos \theta = (1 - t^2)/(1 + t^2) \) and \( \sin \theta = 2t/(1 + t^2) \). Combining them with the resultant method, \( t \) can be eliminated and the constraint equation of the aGBZ Eq. 7 can be finally obtained [74].

\[
F_{\text{aGBZ}}(\beta, \text{Im } \beta) = R^{f,f^g}_\theta(\beta, \text{Im } \beta).
\]

The mathematical meaning of aGBZ is that for a given point \( \beta_0 \) on it with \( f(\beta_0, E_0) = 0 \), there must also exist a conjugate point \( \beta_0 = \beta_0 e^{i\theta_0} \) satisfying \( f(\beta_0, E_0) = 0 \) on it. In general, \( \beta_0 \) and \( \bar{\beta}_0 \) are different points on the aGBZ.

**Analytic arcs on the aGBZ** — Through the above calculation, \( F_{\text{aGBZ}}(\beta, \text{Im } \beta) \) must be a real algebraic polynomial of \( \text{Re } \beta \) and \( \text{Im } \beta \). It is analytic in the entire \( \beta \)-\( \text{Im } \beta \)-plane except for the original point (pole) and the bifurcation (or singularity) point, which is defined by

\[
F_{\text{aGBZ}}(\beta, \text{Im } \beta) = \nabla F_{\text{aGBZ}}(\beta, \text{Im } \beta) = 0,
\]

where \( \nabla = (\partial_{\text{Re } \beta}, \partial_{\text{Im } \beta}) \). Intuitively, these bifurcation points correspond to the self-intersection points on the aGBZ. Hence the aGBZ is constituted by a set of analytic arcs \( \Gamma \) joined by the bifurcation points. Notice that any point on the aGBZ can be labeled by its ordering number, for example, \((j, j + 1)\) represents \( |\beta_j| = |\beta_{j+1}| \), where \( j = 1, \ldots, p + s - 1 \). Furthermore, this number can not be changed in each analytic arc in the aGBZ, since the transition of the ordering can only occur at the bifurcation points. Hence one can label the corresponding ordering to each analytic arc. Finally, we obtain an equivalent GBZ condition in the language of geometry based on the aGBZ. For the real algebraic curve determined by the aGBZ equation \( F_{\text{aGBZ}}(\beta, \text{Im } \beta) = 0 \), one can first label the ordering for each analytic arc. Then, the GBZ is constituted by all the arcs labeled by \((p, p + 1)\). There exist a set of self-conjugate points on the aGBZ, satisfying \( \bar{\beta} = \beta \), which are equivalent to

\[
f(\beta, E) = \partial_{\text{Re } \beta} f(\beta, E) = 0.
\]
A powerful statement about the self-conjugate point is that any analytic arcs containing the self-conjugate points satisfying \( \beta_p = \beta_{p+1} \) must form the GBZ, where \( p \) is the order of the pole. Through the above discussion, one can notice that the aGBZ is a minimal analytic element containing all the informations of GBZ and the GBZ is in general a subset of aGBZ.

Based on the concept of aGBZ and the corresponding geometrical intuition, one can explain and understand the following two perplexing facts: (i) why \( \beta_p \) and \( \beta_{p+1} \) play the special role, namely, determining the GBZ; (ii) why the GBZ satisfying \( |\beta_p| = |\beta_{p+1}| \) must be closed loops.

Let’s take a single-band model as an example, whose characteristic equation can be written as \( E = \sum_{i=-p}^{p} c_i \beta^i \). If all the parameters are finite, the corresponding eigenvalues should also be finite. The GBZ condition \( |\beta_p| = |\beta_{p+1}| \) can be understood as the forbidden of \( E \) tending to infinity for finite parameters. Now we will explain this. From the characteristic equation, in the \( E \rightarrow \infty \) limit, on the one hand \( |\beta_i| \rightarrow 0 \) for \( i = 1,...,p \), on the other hand \( \beta_j \rightarrow \infty \) for \( j = p+1,...,p+s \). Their absolute values tend to be degenerate in the \( E \rightarrow \infty \) limit. However, it is impossible to have \( |\beta_p| = |\beta_{p+1}| \) in the \( E \rightarrow \infty \) limit, since \( |\beta_p| \rightarrow 0 \) and \( |\beta_{p+1}| \rightarrow \infty \). This forbids the energy running to infinity with finite parameters. This explains why \( \beta_p \) and \( \beta_{p+1} \) are so special. For the second fact, we start from the analytic arcs on aGBZ. The arcs satisfying \( |\beta_p| = |\beta_{p+1}| \) must form a continues line for a single band model. This line either goes to infinity, or forms closed loops as shown in Fig. 1. Since \( E \) is finite, \( \beta_p/\beta_{p+1} \) is also finite. Therefore the GBZ must form a closed loop.

**Single band**— Now we use the above method to calculate the GBZ for the following model

\[
\mathcal{H}(\beta) = -1/6 - 1/(2\beta^3) + 8/(5\beta^2) + 10/(3\beta) + 4\beta + 2\beta^2 + \beta^3
\]

Since the order of the pole of the characteristic polynomial is 3, the GBZ is determined by \( |\beta_3| = |\beta_4| \). Fig. 1 (a) shows the corresponding aGBZ, where different color arcs are denoted by their respective orderings. The GBZ is constituted by the red arcs with ordering (3,4) since the order of the pole is 3. A striking feature of this example is that the GBZ can have self-intersection points, as shown in Fig. 1 (a) with the path \( \Gamma_2 - \Gamma_3 - \Gamma_4 - \Gamma_5 \). This feature can be hardly verified by the numerical calculation \cite{74}. The arcs \( \Gamma_{1,6/7} \) are self-conjugate arcs, which means both \( \beta_0 \) and \( \beta_0 \) are one it. The other arcs \( \Gamma_{2,3/4/5} \) and their conjugate arcs \( \tilde{\Gamma}_{2/3/4/5} \) (which are not plotted in Fig. 1) are symmetric along the Re\( \beta \)-axes. Hence if we goes along the GBZ as \( \Gamma_1 - \Gamma_2 - \Gamma_3 - \Gamma_4 - \Gamma_5 - \Gamma_6 - \tilde{\Gamma}_5 - \tilde{\Gamma}_4 - \tilde{\Gamma}_3 - \Gamma_2 - \Gamma_1 \), all the points on the energy spectra will be covered twice as shown in Fig. 1 \cite{30}. The comparisons with the numerical results are shown in the Supplemental Material \cite{74}.

**Multi-band**— For the multi-band system, the characteristic equation \( f(\beta,E) = \prod_{\mu=1}^{n} [E - E_\mu(\beta)] = 0 \) defines a Riemann surface in \( \mathbb{C}^2 \), whose Riemann sheets are determined by its roots \( E_\mu(\beta) \). The band structure with different boundary conditions can be viewed as a set of closed loops on the Riemann surface. For example, under the periodic boundary condition, the BZs for each band are degenerate to the unit circle \( \beta_{BZ,1} = ... = \beta_{BZ,m} = e^{ik} \); and the Bloch band \( E_\mu(\beta_{BZ,\mu}) \) maps the unit circle to a set of closed loops on each Riemann sheet if the BZ does not wind around any branch point. From the periodic boundary condition to the open boundary condition, the loop on each Riemann sheet may change dramatically from \( E_\mu(\beta_{BZ,\mu}) \) to \( E_\mu(\beta_{GBZ,\mu}) \). In general, the sub-G Bloch bands for each band can be non-degenerate in the complex \( \beta \)-plane; and the GBZ band is a mapping from \( \{ \beta_{GBZ,1},...,\beta_{GBZ,m} \} \) to \( \{ E_1(\beta_{GBZ,1}),...,E_m(\beta_{GBZ,m}) \} \) on each Riemann sheet determined by \( E - E_\mu(\beta) = 0 \) with \( \mu = 1,...,m \). Previously, we have mentioned that the multi-band GBZ can be calculated from \( |\beta_p| = |\beta_{p+1}| \). Now we show how can we determine the sub-GBZs for every band from the aGBZ. Notice that for a given \( E_0 \), the solution of \( f(\beta,E_0) = 0 \) is equivalent to \( E_\mu(\beta) = E_0 \) for \( \mu = 1,...,m \). Thus the solutions shown in Eq. 3 can be further assigned to a band index \( \mu \). This means that all the analytic arcs on the aGBZ can not only be labeled by their orderings, but also by their band indexes. By picking up all the \( (p,p+1) \) arcs, the corresponding sub-GBZs are also fixed.

Now we will show an example to illustrate the above procedure with the following Hamiltonian

\[
\mathcal{H}(\beta) = \begin{pmatrix}
    t_0 + t_{-1}/\beta + t_1\beta/c & c \\
    c & w_0 + w_{-1}/\beta + w_1\beta
\end{pmatrix}.
\]

Without loss of generality, we can assume all the parameters are real. The eigenvalues of the Hamiltonian are

\[
E_\pm = h_0(\beta) \pm \sqrt{c^2 + h_2^2(\beta)},
\]

where \( h_0/\pm(\beta) = |h_1(\beta) \pm h_2(\beta)|/2 \), \( h_1(\beta) = t_0 + t_{-1}/\beta +

![Fig. 1](image_url). The aGBZ, GBZ, and a part of energy spectra for the model \( E = -1/6 - 1/(2\beta^3) + 8/(5\beta^2) + 10/(3\beta) + 4\beta + 2\beta^2 + \beta^3 \). In (a), the color of the arcs on the aGBZ indicates the ordering of the arcs. The GBZ is constituted by the red ones labeled by (34) since the order of the pole in this model is 3.
t_1\beta, \ h_2(\beta) = w_0 + w_{-1}/\beta + w_1\beta, \text{ and } t_i \neq -w_i. \ If \ c = 0, \ Eq. 12 \ describes \ two \ independent \ bands \ h_1(\beta) \ and \ h_2(\beta). \ Under \ the \ open \ boundary \ condition, \ the \ spectra \ for \ them \ are \ \epsilon_1(k) = t_0 + 2\sqrt{t_1t_{-1}} \cos k \ and \ \epsilon_2(k) = w_0 + 2\sqrt{w_1w_{-1}} \cos k \ with \ different \ sub-GBZs \ \beta_{GBZ,1} = \sqrt{t_{-1}/t_1}e^{ik} \ and \ \beta_{GBZ,2} = \sqrt{w_{-1}/w_1}e^{ik} [74]. \ Notice \ that \ in \ this \ case, \ the \ characteristic \ equation \ f(\beta, E) = |E - h_1(\beta)||E - h_2(\beta)| \ is \ a \ reducible \ polynomial \ with \ respect \ to \ E. \ The \ asymptotic \ solutions \ are \ determined \ by \ the \ two \ separated \ irreducible \ polynomials \ E - h_1(\beta) \ and \ E - h_2(\beta), \ which \ result \ two \ independent \ sub-GBZs. \ If \ c \neq 0, \ these \ two \ bands \ will \ be \ coupled \ together \ and \ the \ asymptotic \ solutions \ are \ determined \ by \ the \ irreducible \ polynomial \ equation \ f(\beta, E) = |E - h_1(\beta)||E - h_2(\beta)| - c^2. \ Since \ the \ order \ of \ the \ pole \ of \ f(\beta, E) \ is \ 2, \ the \ GBZ \ is \ constituted \ by \ the \ arcs \ with \ ordering (2, 3) \ on \ the \ aGBZ. \ As \ shown \ in \ Fig. 2 (a1) \ and \ (c1), \ all \ the \ arcs \ on \ the \ aGBZ \ can \ be \ labeled \ by \ their \ orderings \ and \ band \ indexes. \ (red \ for \ E_+ \ and \ blue \ for \ E_-). \ The \ (2, 3) \ arcs \ form \ two \ distinct \ closed \ loops, \ which \ correspond \ two \ sub-GBZs \ \beta_{GBZ,1}. \ Any \ arcs \ containing \ the \ degenerate \ points \ satisfying \ \beta_2 = \beta_3 \ (red \ points) \ must \ form \ the \ GBZ. \ The \ spectra \ determined \ by \ E_\pm(\beta_{GBZ,\pm}) \ are \ shown \ in \ Fig. 2 (a2) \ and \ (c2). \ As \ a \ comparison, \ we \ also \ plot \ the \ numerical \ results \ (gray \ points) \ in \ Fig. 2 (a) \ and \ (c), \ whose \ size \ is \ proportional \ to |Im E|. \ The \ parameters \ for \ (a), \ (b) \ and \ (c), \ (d) \ are \ chosen \ to \ be \ t_0 = 4, t_1 = t_{-1} = 1, w_0 = -2, w_1 = 3, w_{-1} = 1, c = -1 \ and \ t_0 = 1, t_1 = 1, t_{-1} = 2, w_0 = -1, w_1 = 3, w_{-1} = 1, c = -1. \n
In Fig. 2 (b) and (d), we plot the Riemann surface determined by \( f(\beta, E) = 0 \) in (Re \beta, Im \beta, Re E) space, where the black points/lines represent the branch points/cuts. Different colors represent different Riemann sheets (red for \( E_+ \) and blue for \( E_- \)). We also plot the band structure of GBZ \( E_\pm(\beta_{GBZ,\pm}) \) on the Riemann surface with red and blue lines. It can be realized that although the two sub-GBZs in Fig. 2 (c1) have intersection points, their GBZ bands are separated as shown in Fig. 2 (d), since the two sub-GBZs do not cross the branch cut, they are separated bands. We finally note that for a given \( E \) away from the Re E-axes in Fig. 2 (c2), the asymptotic eigenstate is the superposition of the generalized Bloch waves belonging to different bands.

Discussion and conclusion—The multi-band non-Hermitian systems are slightly different from single-band model, although they share the same GBZ condition \( |\beta_p| = |\beta_{p+1}| \) if all the bands are coupled together. It has been shown \[31, 55\] that the winding of \( E \) for single-band model must be zero under the open boundary condition. Here we conjecture that the total winding of \( E \) for multi-band system should be zero as a direct generalization of the single-band result. The existence of non-degenerate sub-GBZs implies: (i) the winding number of energy expressed by \( \det[\mathcal{H}(\beta) - E\mathbb{I}] \) can not be applied directly, since the integral path for different bands are distinct; (ii) the \( \beta \)-dependent term \( h_0(\beta)I_m \times m \) can not be omitted for the non-Hermitian systems, since the open boundary spectrum of \( \mathcal{H}(\beta) \) and \( h_0(\beta)I_m \times m + \mathcal{H}(\beta) \) can be totally different; (iii) the dispersion relation of...
non-Hermitian multi-band system is a mapping from \( \{ \beta_{GBZ,1}, \ldots, \beta_{GBZ,m} \} \) to \( \{ E_1(\beta_{GBZ,1}), \ldots, E_m(\beta_{GBZ,m}) \} \), which correspond to different loops on the Riemann surface determined by the characteristic equation.

In summary, we have provided a systematic method to calculate the GBZ analytically based on the concept of a GBZ in non-Hermitian systems. For the multi-band systems, we have shown that the GBZ can be several non-degenerate piecewise analytic closed loops. The generalization of GBZ condition for other symmetry classes is left for the further study.

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1 C. M. Bender, Rep. Prog. Phys. 70, 947 (2007).
2 N. Moiseyev, Non-Hermitian Quantum Mechanics (Cambridge University Press, 2011).
3 I. Rotter and J. P. Bird, Rep. Prog. Phys. 78, 114001 (2015).
4 L. Feng, R. El-Ganainy, and L. Ge, Nat. Photonics 11, 752 (2017).
5 R. El-Ganainy, K. G. Makris, M. Khajavikhan, Z. H. Musslimani, S. Rotter, and D. N. Christodoulides, Nat. Phys. 14, 11 (2018).
6 S. K. Özdemir, S. Rotter, F. Nori, and L. Yang, Nat. Mater. 18, 783 (2019).
7 M.-A. Miri and A. Ali, Science 363, eaar7709 (2019).
8 S. K. Gupta, Y. Zou, X.-Y. Zhu, M.-H. Lu, L. Zhang, X.-P. Liu, and Y.-F. Chen, (2018), arXiv:1803.00794.
9 V. M. Martinez Alvarez, J. E. Barrios Vargas, M. Berdakin, and L. E. F. Foa Torres, Eur. Phys. J. Spec. Top. 227, 1295 (2018).
10 A. Ghatak and T. Das, J. Phys.: Condens. Matter 31, 263001 (2019).
11 C. M. Bender and S. Boettcher, Phys. Rev. Lett. 80, 5243 (1998).
12 C. M. Bender, D. C. Brody, and H. F. Jones, Phys. Rev. Lett. 89, 270401 (2002).
13 M. A. Stephano, Phys. Rev. Lett. 76, 4472 (1996).
14 N. Hatano and D. R. Nelson, Phys. Rev. Lett. 77, 570 (1996).
15 M. S. Rudner and L. S. Levitov, Phys. Rev. Lett. 102, 065703 (2009).
16 S. Longhi, Phys. Rev. Lett. 105, 013903 (2010).
17 T. E. Lee, Phys. Rev. Lett. 116, 133903 (2016).
18 D. Leykam, K. Y. Bloch, C. Huang, Y. D. Chong, and F. Nori, Phys. Rev. Lett. 118, 040401 (2017).
19 R. A. Molina and J. González, Phys. Rev. Lett. 120, 146601 (2018).
20 V. Koizzi and L. Fu, arXiv e-prints , arXiv:1708.05841 (2017), arXiv:1708.05841 [cond-mat.mes-hall].
21 M. Papaj, H. Isole, and L. Fu, Phys. Rev. B 99, 201107 (2019).
22 H. Shen, B. Zhen, and L. Fu, Phys. Rev. Lett. 120, 146402 (2018).
23 H. Shen and L. Fu, Phys. Rev. Lett. 121, 026403 (2018).
24 S. Yao and Z. Wang, Phys. Rev. Lett. 121, 086803 (2018).
25 S. Yao, F. Song, and Z. Wang, Phys. Rev. Lett. 121, 136802 (2018).
26 F. Song, S. Yao, and Z. Wang, Phys. Rev. Lett. 123, 170401 (2019).
27 F. Song, S. Yao, and Z. Wang, Phys. Rev. Lett. 123, 246801 (2019).
28 F. K. Kunst, E. Edvardsson, J. C. Budich, and E. J. Bergholtz, Phys. Rev. Lett. 121, 026808 (2018).
29 K. Yokomizo and S. Murakami, Phys. Rev. Lett. 123, 066404 (2019).
30 K. Zhang, Z. Yang, and C. Fang, arXiv:1910.01131.
31 N. Okuma, K. Kawabata, K. Shiozaki, and M. Sato, arXiv:1910.02878.
32 Y. Xu, S.-T. Wang, and L.-M. Duan, Phys. Rev. Lett. 118, 045701 (2017).
33 A. Cerjan, M. Xiao, L. Yuan, and S. Fan, Phys. Rev. B 97, 075128 (2018).
34 B. Carlström and E. J. Bergholtz, Phys. Rev. A 98, 042114 (2018).
35 Z. Yang and J. Hu, Phys. Rev. B 99, 081102 (2019).
36 K. Kawabata, T. Bessho, and M. Sato, Phys. Rev. Lett. 123, 066405 (2019).
37 Z. Yang, A. P. Schuender, J. Hu, and C.-K. Chiu, arXiv e-prints , arXiv:1912.02788 (2019), arXiv:1912.02788 [cond-mat.mes-hall].
38 T. Liu, Y.-R. Zhang, Q. Ai, Z. Gong, K. Kawabata, M. Ueda, and F. Nori, Phys. Rev. Lett. 122, 076801 (2019).
39 Z. Zhang, M. Rosendo López, Y. Cheng, X. Liu, and J. Christensen, Phys. Rev. Lett. 122, 195501 (2019).
40 X.-W. Luo and C. Zhang, Phys. Rev. Lett. 123, 073601 (2019).
41 C. H. Lee, L. Li, and J. Gong, Phys. Rev. Lett. 123, 016805 (2019).
42 Z. Gong, Y. Ashida, K. Kawabata, K. Takasan, S. Higashikawa, and M. Ueda, Phys. Rev. X 8, 031079 (2018).
43 H. Zhou and J. Y. Lee, Phys. Rev. B 99, 235112 (2019).
44 K. Kawabata, K. Shiozaki, M. Ueda, and M. Sato, Phys. Rev. X 9, 041015 (2019).
45 C.-H. Liu, H. Jiang, and S. Chen, Phys. Rev. B 129, 25103 (2019).
46 J. Y. Lee, J. Ahn, H. Zhou, and A. Vishwanath, Phys. Rev. Lett. 123, 206404 (2019).
47 R. Hamazaki, K. Kawabata, and M. Ueda, Phys. Rev. Lett. 123, 090603 (2019).
48 S. Longhi, Phys. Rev. Lett. 122, 237601 (2019).
49 B. Höckendorf, A. Alvermann, and H. Fehske, Phys. Rev. Lett. 123, 190403 (2019).
50 Y. Xiong, J. Phys. Commun. 2, 035043 (2018).
51 V. M. Martinez Alvarez, J. E. Barrios Vargas, and L. E. F. Foa Torres, Phys. Rev. B 99, 121401 (2018).
52 C. H. Lee and R. Thomale, Phys. Rev. B 99, 201103 (2019).
53 S. Longhi, arXiv:1909.06211.
54 L. Herviou, J. H. Bardarson, and N. Regnault, Phys. Rev. A 99, 052118 (2019).
55 H.-G. Zirnstein, G. Refael, and B. Rosenow,
[56] H. Jiang, L.-J. Lang, C. Yang, S.-L. Zhu, and S. Chen, Phys. Rev. B 100, 054301 (2019), arXiv:1901.09399.

[57] S. Longhi, Phys. Rev. Research 1, 023013 (2019).

[58] K.-I. Imura and Y. Takane, Phys. Rev. B 100, 165430 (2019).

[59] T. Helbig, T. Hofmann, S. Imhof, M. Abdelghany, T. Kiessling, L. W. Molenkamp, C. H. Lee, A. Szameit, M. Greiter, and R. Thomale, arXiv e-prints, arXiv:1907.11562 (2019), arXiv:1907.11562 [cond-mat.mes-hall].

[60] T. Helbig, T. Hofmann, S. Imhof, M. Abdelghany, T. Kiessling, L. W. Molenkamp, C. H. Lee, A. Szameit, M. Greiter, and R. Thomale, “Observation of bulk boundary correspondence breakdown in topolectrical circuits,” (2019), arXiv:1907.11562.

[61] L. Xiao, T. Deng, K. Wang, G. Zhu, Z. Wang, W. Yi, and P. Xue, arXiv e-prints, arXiv:1907.12566 (2019), arXiv:1907.12566 [cond-mat.mes-hall].

[62] T. Hofmann, T. Helbig, F. Schindler, N. Salgo, M. Brazzińska, M. Greiter, T. Kiessling, D. Wolf, A. Vollhardt, A. Kabasî, C. H. Lee, A. Bílišić, R. Thomale, and T. Neupert, arXiv e-prints, arXiv:1908.02759 (2019), arXiv:1908.02759 [cond-mat.mes-hall].

[63] X. Zhang and J. Gong, arXiv e-prints, arXiv:1909.10234 (2019), arXiv:1909.10234 [cond-mat.mes-hall].

[64] L. Li, C. H. Lee, and J. Gong, arXiv e-prints, arXiv:1910.03229 (2019), arXiv:1910.03229 [cond-mat.mes-hall].

[65] L. E. F. F. Torres, Journal of Physics: Materials 3, 014002 (2019).

[66] D. S. Borgnia, A. J. Kruchkov, and R.-J. Slager, arXiv:1902.07217.

[67] W. Brzezicki and T. Hyart, Phys. Rev. B 100, 161105 (2019).

[68] T.-S. Deng and W. Yi, Phys. Rev. B 100, 035102 (2019).

[69] E. Edvardsson, F. K. Kunst, and E. J. Bergholtz, Phys. Rev. B 99, 081302 (2019).

[70] M. Ezawa, Phys. Rev. B 99, 121411 (2019).

[71] F. K. Kunst and V. Dwivedi, Phys. Rev. B 99, 245116 (2019).

[72] H. Wang, J. Ruan, and H. Zhang, Phys. Rev. B 99, 075130 (2019).

[73] A. Alase, E. Cobanera, G. Ortiz, and L. Viola, Phys. Rev. Lett. 117, 076804 (2016).

[74] See Supplemental Material for details.

[75] M. J. Colbrook, B. Roman, and A. C. Hansen, Phys. Rev. Lett. 122, 250201 (2019).

[76] Wikipedia (2019), page Version ID: 905762282.

[77] H. Woody, Polynomial Resultants, 10 (2016).

[78] S. Janson, RESULTANT AND DISCRIMINANT OF POLYNOMIALS, 18 (2010).

[79] I. M. Gelfand, M. Kapranov, and A. Zelevinsky, Discriminants, Resultants, and Multidimensional Determinants (Springer Science & Business Media, 2008).
Supplemental Material for
“Auxiliary generalized Brillouin zone method in non-Hermitian band theory”

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I. AN EXACT SOLVABLE MODEL

In this section, we will use an exact solvable model to illustrate the procedure of exact solution for a finite size
lattice system with open boundary condition. Consider the following Hamiltonian with arbitrary boundary condition

\[
\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{H}_B,
\]

\[
\hat{H}_0 = \sum_{i=1}^{N-1} (t_1 \hat{c}_i^\dagger \hat{c}_{i+1} + t_{-1} \hat{c}_{i+1}^\dagger \hat{c}_i),
\]

\[
\hat{H}_B = t_{-1} \hat{c}_1^\dagger \hat{c}_N + t_1 \hat{c}_N^\dagger \hat{c}_1,
\]

where \(\hat{H}_0\) is the open boundary Hamiltonian and \(N\) denotes the number of sites of the one dimensional chain. In order
to simplify the discussion, we can assume that \(t_{\pm 1}\) are real positive numbers without loss of generality. If \(t_1 = t_{-1}^*\)
and \(\lambda \in \mathbb{R}\), \(\hat{H}(\lambda)\) is Hermitian, otherwise, it is non-Hermitian. The eigenequation of the Hamiltonian in Eq. (1) can

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be written as the following matrix form,
\[
\begin{pmatrix}
0 & t_1 & 0 & \ldots & 0 & \lambda t_{-1} \\
t_{-1} & 0 & t_1 & \ldots & 0 & 0 \\
0 & t_{-1} & 0 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ldots & 0 & t_1 \\
\lambda t_1 & 0 & 0 & \ldots & t_{-1} & 0 \\
\end{pmatrix}
\begin{pmatrix}
\phi_1 \\
\phi_2 \\
\phi_3 \\
\vdots \\
\phi_{N-1} \\
\phi_{N} \\
\end{pmatrix}
= E
\begin{pmatrix}
\phi_1 \\
\phi_2 \\
\phi_3 \\
\vdots \\
\phi_{N-1} \\
\phi_{N} \\
\end{pmatrix}
\]
(2)

where \( \Phi = (\phi_1, ..., \phi_N)^\dagger \) represents the non-normalized eigenfunction of \( \hat{H}(\lambda) \).

### A. Open boundary \((\lambda = 0)\) solution

If \( \lambda = 0 \), the Hamiltonian reduces to the case of open boundary. The procedure to obtain the solution is similar to the case of solving the infinite square well problem, where we first solve the (bulk) Schrödinger equation \(-\hbar^2 \partial_x^2 \phi(x) = 2m(E - V_0)\phi(x)\) and eigenstates can be expressed as the superposition of (bulk) solutions \( \phi(x) = e^{\pm ikx} \) such as the boundary condition is satisfied.

Based on the same method, the recursive bulk equation can be obtained from Eq. (2),
\[
t_{-1}\phi_{i-1} + t_1\phi_{i+1} = E\phi_i,
\]
(3)

where \( i = 2, ..., N - 1 \). We first solve the bulk equation. Notice that Eq. (3) has discrete translational symmetry. This implies the bulk solution can be written as \( \Phi(\beta) = (\beta_1, \beta_2, ..., \beta_N)^\dagger \). Putting this solution into Eq. (3), the bulk equation becomes
\[
t_1\beta^2 - E\beta + t_{-1} = 0.
\]
(4)

Hence, for a given \( E \), there exist two bulk solutions, \( \Phi_E(\beta_1) \) and \( \Phi_E(\beta_2) \), where
\[
\beta_{1/2} = \frac{E \pm \sqrt{E^2 - 4t_1t_{-1}}}{2t_1}.
\]
(5)

Next, the discussion can be classified by the following two cases.

*(a) \( \beta_1 \neq \beta_2 \)* case

If \( \beta_1 \neq \beta_2 \), the solution of Eq. 2 with eigenvalue \( E \) can be written as the superposition of the above two bulk solutions, namely,
\[
\Phi_E = c_1\Phi_E(\beta_1) + c_2\Phi_E(\beta_2).
\]
(6)

Putting Eq. (6) into Eq. (2), one can obtain the following constraint of boundary condition
\[
t_1(c_1\beta_1^2 + c_2\beta_2^2) = E(c_1\beta_1 + c_2\beta_2),
\]
\( t_{-1}(c_1\beta_1^{N-1} + c_2\beta_2^{N-1}) = E(c_1\beta_1^N + c_2\beta_2^N). \)
(7)

By solving this boundary condition, one can obtain a set of quantized \( \beta \) and \( E \) for a finite size system. Using the bulk equation Eq. (4), the above boundary condition Eq. (7) can be rewritten as the following matrix form,
\[
\begin{pmatrix}
t_1\beta_1^2 - (t_{-1} + t_1\beta_1^2) \\
t_{-1}\beta_1^{N-1} - (t_{-1}\beta_1^{N-1} + t_1\beta_1^{N+1}) \\
\end{pmatrix}
\begin{pmatrix}
t_1\beta_2^2 - (t_{-1} + t_1\beta_2^2) \\
t_{-1}\beta_2^{N-1} - (t_{-1}\beta_2^{N-1} + t_1\beta_2^{N+1})
\end{pmatrix}
\begin{pmatrix}
c_1 \\
c_2
\end{pmatrix}
= \begin{pmatrix}
-t_{-1} \\
-t_{-1}
\end{pmatrix}
\begin{pmatrix}
c_1 \\
c_2
\end{pmatrix}
= 0.
\]
(8)

The nontrivial solutions require the determinant of the coefficient matrix vanish, namely,
\[
t_1t_{-1}(\beta_2^{N+1} - \beta_1^{N+1}) = 0.
\]
(9)

Using the condition \( \beta_1\beta_2 = t_{-1}/t_1 \) from Eq. (4), one can obtain
\[
(t_{-1}/t_1)^{N+1} - \beta_1^{2N+2} = 0,
\]
(10)
where $\beta_{1/2}$ represents $\beta_1$ and $\beta_2$. By solving the above equation, one can obtain the following quantized $\beta_{1/2}$

$$\beta_{1/2} = \left(\frac{t_{-1}}{t_1}\right)^{1/2} e^{ik}, \quad \beta_{2/1} = \left(\frac{t_{-1}}{t_1}\right)^{1/2} e^{-ik},$$

and $E$,

$$E = t_0 + 2\sqrt{t_1 t_{-1}} \cos k,$$

where

$$k = \frac{\pi m}{N + 1}, \quad m = 1, ..., N$$

Notice that $m \neq 0, \pm(N + 1)$, since we forbid the case $\beta_1 = \beta_2$.

(b) $\beta_1 = \beta_2$ case

If $\beta_1 = \beta_2$, the solution can not be written as the form of Eq. (6). According to Eq. (5), $\beta_1 = \beta_2$ requires

$$E_c = t_0 \pm 2\sqrt{t_1 t_{-1}},$$

and

$$\beta_c = \beta_1 = \beta_2 = \pm \sqrt{t_{-1}/t_1} = \sqrt{t_{-1}/t_1} e^{i k_c},$$

where $k_c = 0, \pm \pi$. If $N$ is finite, this bulk wave function $\Phi_{E_c}(\beta_c)$ do not satisfy the boundary condition Eq. (7). However, if $N \to \infty$, there exist two different cases: (i) $|\beta| = 1$, namely the Hermitian case ($t_{-1} = t_1$ since we have already assumed $t_{\pm 1}$ are real positive numbers), the bulk solution $\Phi_{E_c}(\beta_c) = e^{i k_c x}$ is the Bloch wave function, which becomes the asymptotic solution in the $N \to \infty$ limit; (ii) $|\beta| \neq 1$, which is the non-Hermitian case ($t_{-1} \neq t_1$), the bulk solution $\Phi_{E_c}(\beta_c) = \sqrt{t_{-1}/t_1} e^{i k_c x}$ will be divergent at the infinity boundary. Hence, they can not be the (bounded) asymptotic solutions.

By solving the coefficients $c_1$ and $c_2$ from Eq. (8), The eigenfunctions can be obtained

$$\Phi_E \propto \Phi_{E_c}(\beta_1) - \Phi_{E_c}(\beta_2) \propto (\phi_1, ..., \phi_N)^t,$$

with

$$\phi_m = \left(\frac{t_{-1}}{t_1}\right)^{m/2} \sin km,$$

where $k = m \pi/(N + 1)$ and $m = 1, ..., N$. If $t_1 \neq t_{-1}$, all the eigenstates of the Hamiltonian will be localized at one of the boundary of the lattice chain. These eigenstates are dubbed as non-Hermitian skin modes [1].

B. Periodic boundary ($\lambda = 1$) solution

As a comparison, we use the same method to solve Eq. (2) with periodic boundary condition, namely, $\lambda = 1$. It can be shown, the boundary condition in this case becomes

$$\mathcal{M}_B \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 1 - \beta_1^N \\ \beta_1(1 - \beta_1^N) \end{pmatrix} \begin{pmatrix} 1 - \beta_2^N \\ \beta_2(1 - \beta_2^N) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0.$$

One can notice the boundary condition is independent of the parameter. The condition for the vanishing of the determinant of the coefficient matrix can be written as

$$(\beta_1 - \beta_2)(1 - \beta_1^N)(1 - \beta_2^N) = 0.$$

This equation requires

$$\beta_{1/2} = e^{ik}, \quad k = \frac{2\pi m}{N},$$

A little difference occurs between the Hermitian and non-Hermitian case.
(a). $t_1 = t_{-1}$ case

In this Hermitian case, according to $\beta_1 \beta_2 = t_{-1}/t_1 = 1$, both $\Psi_E(\beta_1)$ and $\Psi_E(\beta_2)$ are the solutions. And any linear superposition of them is also the solution.

(b). $t_1 \neq t_{-1}$ case

In this non-Hermitian case, according to $\beta_1 \beta_2 = t_{-1}/t_1 \neq 1$, either $\Psi_E(\beta_1)$ or $\Psi_E(\beta_2)$ is the solutions. Their linear superposition $c_1 \Psi_E(\beta_1) + c_2 \Psi_E(\beta_2)$ is not the solution. This means for a give energy, there only exist one eigenstates in the case of periodic boundary condition. It has been shown that this implies the nontrivial winding of energy and the failure of conventional bulk-boundary correspondence [2, 3].

II. GBZ CONDITION

The condition of GBZ has been first explored in Ref [1, 4] with chiral symmetry and in Ref [2] with general single band models. Here we generalize the condition of GBZ to arbitrary multi-band models without any symmetry or with chiral symmetry.

Consider a general $m$–band 1D Hamiltonian in real space

$$\hat{H} = \sum_{i,j=1}^{N} \sum_{\mu,\nu=1}^{m} t_{ij}^{\mu\nu} \hat{c}_i^\dagger \hat{c}_j^\nu,$$

where $t_{ij}^{\mu\nu} \neq (t_{ji}^{\nu\mu})^*$ and $i,j$ and $\mu,\nu$ label the lattice sites and band indexes respectively.

Firstly, the characteristic equation can be written as

$$f(\beta, E) = \det[\hat{H}(\beta) - E\hat{I}] = \sum_{i=-p}^{s} \sum_{j=0}^{m} c_{ij}\beta^i E^j = 0,$$

where $[\hat{H}(\beta)]_{\mu\nu} = \sum_{i=-1}^{N} t_{i}^{\mu\nu} \beta^i$, $t_{i}^{\mu\nu} = t_{ij}^{\nu\mu} \delta_{i+1,j}$, and $\beta = e^{ik}$ labeling the Bloch wave with the complex wave-vector $k$.

Secondly,

- if $f(\beta, E)$ is an irreducible algebraic polynomial, we can solve the characteristic equation for a given $E$, and order the solutions by the absolute value as

$$|\beta_1(E)| \leq |\beta_2(E)| \leq \ldots \leq |\beta_{p+1}(E)|. $$

Finally, if $|\beta_p(E)| = |\beta_{p+1}(E)|$, where $p$ is the order of the pole in Eq. (22), then, $E$ is an eigenvalue of $\hat{H}$ in the thermodynamic limit $N \rightarrow \infty$.

- if $f(\beta, E)$ is an reducible algebraic polynomial, which can be written as

$$f(\beta, E) = \prod_{i=1}^{n} f_i(\beta, E),$$

where $f_i(\beta, E)$ is irreducible algebraic polynomial, then, for every $i = 1, \ldots, n$ we can solve $f_i(\beta, E) = 0$ for a given $E$, and order the corresponding solutions by the absolute value as

$$|\beta_{i,1}(E)| \leq |\beta_{i,2}(E)| \leq \ldots \leq |\beta_{i,p_i}(E)|. $$

Finally, if $|\beta_{i,p_i}(E)| = |\beta_{i,p_i+1}(E)|$, where $p_i$ is the order of the pole in $f_i(\beta, E)$, then, $E$ is an eigenvalue of $\hat{H}$ in the thermodynamic limit $N \rightarrow \infty$.

The second case of the above discussion applies to the cases where several bands are independent and not be coupled together. The proof for the first case can be found in the Ref [2, 4]. Here we complete the condition in second case, which can be viewed as a generalization of the first case. The example can be found in the main text.
III. CHARACTERISTIC EQUATION OF HERMITIAN CASE

For the Hamiltonian with open boundary condition defined in Eq. 1 in the main text, if the Hamiltonian is Hermitian, it must satisfy

\[ H^* = H^t. \]  

(26)

Here we define

\[ H_1 := H^*, \quad H_2 := H^t \]

(27)

Then, the corresponding bulk Hamiltonians can be written as

\[ [H_1(\beta)]_{\mu\nu} = \sum_{i,j} (t_i^\mu)^* \beta^{-i} = \sum_{i=-l_1}^{l_2} \tau_i^\mu \beta^i, \]

(28)

and

\[ [H_2(\beta)]_{\mu\nu} = \sum_{i,j} \tau_i^\mu \beta^{-i} = \sum_{i=-l_1}^{l_2} \tau_i^\mu \beta^i. \]

(29)

Now, the characteristic equation for the \( H_1 \) and \( H_2 \) becomes

\[ \det[H_1(\beta) - E \hat{1}] = \sum_{i=-p}^{s} \sum_{j=0}^{n} c_{ij} \beta^j E^i = f^*(\beta^*, E) = 0, \]

(30)

and

\[ \det[H_2(\beta) - E \hat{1}] = \sum_{i=-p}^{s} \sum_{j=0}^{m} c_{ij} \beta^{-i} E^j = f(\beta^{-1}, E) = 0, \]

(31)

Here we have used the fact that \( E \in \mathbb{R} \) for the Hermitian case. As a result, we obtain

\[ f^*(\beta^*, E) = f(1/\beta, E) \]

(32)

for the Hermitian Hamiltonian. Notice we want to use the above equation to show that \( C_\beta = e^{ik} \) in the Hermitian case. It is necessary to assume \( \beta^* \neq \beta^{-1} \) in the above derivation.

IV. RESULTANT OF TWO POLYNOMIALS

In the main text, we have mentioned that the aGBZ can be calculated from the resultant of two polynomials. Now we show how can we calculate them.

**Definition A.1** (Polynomial). A polynomial \( f(x) \in F[x] \) is defined as

\[ f(x) = \prod_{i=1}^{n} (x - \xi_i) = a_n x^n + a_{n-1} x^{n-1} + \ldots + a_1 x + a_0, \quad a_n \neq 0 \]

(33)

where each coefficient \( a_i \) belongs to the field \( F \) and each root \( \xi_i \) belongs to the extension of \( F \). For example, if \( a_n, \ldots, a_0 \)

are real numbers, \( \xi_1, \ldots, \xi_n \) are complex numbers.

**Definition A.2** (Resultant). Given two polynomials \( f(x) = a_n x^n + \ldots + a_0, \) \( g(x) = b_m x^m + \ldots + b_0 \in F[x] \), their resultant relative to the variable \( x \) is a polynomial over the field of coefficients of \( f(x) \) and \( g(x) \), and is defined as

\[ R(f, g) = a_n^m b_m^n \prod_{i,j} (\xi_i - \eta_j), \]

(34)

where \( f(\xi_i) = 0 \) for \( 1 \leq i \leq n \) and \( g(\eta_j) = 0 \) for \( 1 \leq j \leq m \).

**Theorem A.3.** Let \( f(x) = a_n x^n + \ldots + a_0, \) \( g(x) = b_m x^m + \ldots + b_0 \in F[x], \)
FIG. 1: The numerical results of Fig. 1 in the main text. Here the lattice size (N) and degrees of precision (P) is chosen to be $N = 2000$ $P = 800$ for the left and $N = 3000$ $P = 1800$ for the right. The calculation time for the right side is 11 days. Notice we still do not know whether there exist self-intersection points through the numerical calculation. Here $\beta_x := \Re \beta$ and $\beta_y := \Im \beta$.

1. Suppose that $f$ has $n$ roots $\xi_1, \ldots, \xi_n$ in some extension of $F$. Then

$$R(f, g) = a_n^m \prod_{i=1}^{n} g(\xi_i).$$

(35)

2. Suppose that $g$ has $m$ roots $\eta_1, \ldots, \eta_m$ in some extension of $F$. Then

$$R(f, g) = (-1)^{mn} b_m^n \prod_{j=1}^{m} f(\eta_j).$$

(36)

The proof can be found in Ref [5, 6].

**Theorem A.4.** Let $f$ and $g$ be two non-zero polynomials with coefficients in a field $F$. Then $f$ and $g$ have a common root in some extension of $F$ if and only if their resultant $R(f, g)$ is equal to zero.

**Proof.** Suppose $\gamma$ is their common root, $R(f, g) \propto (\gamma - \gamma) = 0$. Conversely, if $R(f, g) = 0$, at least one of the factors of $R(f, g)$ must be zero, say $\xi_i - \eta_j = 0$, then, $\xi_i = \eta_j$ is their common root.

From Theorem A.4, the resultant can be applied to make sure whether or not two polynomials share a common root. However, from Definition A.2, the calculation of the resultant requires to know the roots of each polynomial. The following theorem enables us to calculate the resultant directly according to the coefficients of $f$ and $g$.

**Definition A.5.** The Sylvester matrix of two polynomials $f(x) = a_n x^n + \ldots + a_0$, $g(x) = b_m x^m + \ldots + b_0 \in F[x]$ is
defined by

\[
\text{Syl}(f,g) = \begin{pmatrix}
    a_n & a_{n-1} & a_{n-2} & \cdots & 0 & 0 & 0 \\
    0 & a_n & a_{n-1} & \cdots & 0 & 0 & 0 \\
    \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
    0 & 0 & 0 & \cdots & a_1 & a_0 & 0 \\
    0 & 0 & 0 & \cdots & a_2 & a_1 & a_0 \\
    b_m & b_{m-1} & b_{m-2} & \cdots & 0 & 0 & 0 \\
    0 & b_m & b_{m-1} & \cdots & 0 & 0 & 0 \\
    \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
    0 & 0 & 0 & \cdots & b_1 & b_0 & 0 \\
    0 & 0 & 0 & \cdots & b_2 & b_1 & b_0
\end{pmatrix},
\]  

(37)

where \(a_n, \ldots, a_0\) are the coefficients of \(f\) and \(b_m, \ldots, b_0\) are the coefficients of \(g\).

**Theorem A.6.** The resultant of two polynomials \(f, g\) equals to the determinant of their Sylvester matrix, namely

\[
R(f,g) = \det[\text{Syl}(f,g)]
\]

(38)

For example, if \(n = 3, m = 2\),

\[
R(f,g) = \det \begin{pmatrix}
    a_3 & a_2 & a_1 & a_0 \\
    0 & a_3 & a_2 & a_1 & a_0 \\
    b_2 & b_1 & b_0 & 0 & 0 \\
    0 & b_2 & b_1 & b_0 & 0 \\
    0 & 0 & b_2 & b_1 & b_0
\end{pmatrix}.
\]

(39)

The proof the this theorem can be found in Ref [5, 6].

V. NUMERICAL RESULT OF FIG. 1

In this section, we show some additional numerical results of Fig. 1 in the main text. On the left side of Fig. 1, we numerical solve the open boundary Hamiltonian with \(N = 2000\) and 800 degrees of precision in Mathematica. The calculation time is about 3 days. On the right side of Fig. 1, we numerical solve the open boundary Hamiltonian with \(N = 3000\) and 1800 degrees of precision in Mathematica. The calculation time is about 11 days. Even in the right side of Fig. 1, we still do not know whether there exist self-intersection points on the GBZ.

VI. SINGLE BAND MODEL

Here we will provide some additional examples for the single band model, where the characteristic equation is

\[
f(\beta, E) = E - \sum_{m=-p}^{s} t_m \beta^m, \quad j = 1, 2.
\]

(40)

To simplify the discussion, we assume that all the parameters are real. Fig. 2 shows some examples of aGBZ and GBZ. The nonzero parameters are chosen to be \(t_{-2} = 1/5, t_{-1} = 3/2, t_1 = 1\) for (a); \(t_{-2} = 1/5, t_{-1} = 1, t_1 = 1, t_2 = 1/3\) for (b); \(t_{-3} = -1/2, t_{-2} = 1/5, t_{-1} = 3/2, t_1 = 1, t_2 = 1/6\) for (c); \(t_{-3} = -1/2, t_{-2} = 1/5, t_{-1} = 3/2, t_1 = 1, t_2 = 1/6, t_3 = 1/2\) for (d). As a comparison, we also plot the numerical calculation of the GBZ in (a1)-(d1) with the gray points, whose size is proportional to \(|\text{Im} E|\). Any arcs containing the degenerate points satisfying \(\beta_p = \beta_{p+1}\) (red points) must form the GBZ. The eigenvalues are shown in (a2)-(d2).

[1] S. Yao and Z. Wang, Phys. Rev. Lett. 121, 086803 (2018).
[2] K. Zhang, Z. Yang, and C. Fang, arXiv:1910.01131.
[3] N. Okuma, K. Kawabata, K. Shiozaki, and M. Sato, arXiv:1910.02878.
[4] K. Yokomizo and S. Murakami, Phys. Rev. Lett. 123, 066404 (2019).
[5] H. Woody, Polynomial Resultants, 10 (2016).
[6] S. Janson, RESULTANT AND DISCRIMINANT OF POLYNOMIALS, 18 (2010).
FIG. 2: The GBZ, aGBZ and the corresponding open boundary energy spectra of the Hamiltonian determined by the characteristic equation Eq. 40. In (a1)-(d1), the red curves, gray points, and red points represent the aGBZ, numerical calculation of GBZ with \( N = 30 \), and degenerate points satisfying \( \beta_p = \beta_{p+1} \). The size of the dots is proportional to \( |\text{Im} E| \). The analytic arcs containing the red points in the aGBZ must form the GBZ. The energy spectrum with \( N = 30 \) are plotted in the second row. The model is shown in Eq. (40) and the parameters are chosen to be \( t_{-2} = 1/5, t_{-1} = 3/2, t_1 = 1 \) for (a); \( t_{-2} = 1/5, t_{-1} = 1, t_1 = 1, t_2 = 1/3 \) for (b); \( t_{-3} = -1/2, t_{-2} = 1/5, t_{-1} = 3/2, t_1 = 1, t_2 = 1/6 \) for (c); \( t_{-3} = -1/2, t_{-2} = 1/5, t_{-1} = 3/2, t_1 = 1, t_2 = 1/6, t_3 = 1/2 \) for (d).