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Non-Bloch Band Theory of Non-Hermitian Systems

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In spatially periodic Hermitian systems, such as electronic systems in crystals, the band structure is described by the band theory in terms of the Bloch wave functions, which reproduces energy levels for large systems with open boundaries. In this paper, we establish a generalized Bloch band theory in one-dimensional spatially periodic tight-binding models. We show how to define the Brillouin zone in non-Hermitian systems. From this Brillouin zone, one can calculate continuum bands, which reproduce the band structure in an open chain. As an example we apply our theory to the non-Hermitian SSH model. We also show the bulk-edge correspondence between the winding number and existence of the topological edge states.

The band theory in crystals is fundamental for describing electronic structure[1]. By introducing the Bloch wave vector $\boldsymbol{k}$, the band structure calculated within a unit cell reproduces that of a large crystal with open boundaries. Here it is implicitly assumed that the electronic states are almost equivalent between a system with open boundaries and that with the periodic boundaries, represented by the Bloch wave function with real $\boldsymbol{k}$. It is because the electronic states extend over the system.

Recently non-Hermitian systems, which are described by non-Hermitian Hamiltonians have been attracting much attention. These systems have been both theoretically and experimentally studied in many fields of physics[2–71]. In particular, the bulk-edge correspondence has been intensively studied in topological systems. In contrast to Hermitian systems, it seems to be violated in some cases. The reasons for this violation have been under debate[52,72–94].

One of the controversy is that in many previous works, the Bloch wave vector has been treated as real in non-Hermitian systems similarly to Hermitian ones. In Ref. 83, it was proposed that in one-dimensional (1D) non-Hermitian systems, the wave number k becomes complex. The value of $\beta \equiv \mathrm{e}^{ik}$ is confined on a loop on the complex plane, and this loop is a generalization of the Brillouin zone in Hermitian systems. In non-Hermitian systems, the wave functions in large systems with open boundaries do not necessarily extend over the bulk, but are localized at the either end of the chain unlike those in Hermitian systems. This phenomenon is called the non-Hermitian skin effect[83]. Thus far, how to obtain the generalized Brillouin zone has been known only for simple systems.

In this paper, we establish a generalized Bloch band theory in a 1D tight-binding model in the way to determine the generalized Brillouin zone C_β for $\beta \equiv \mathrm{e}^{ik}$, $k \in \mathbb{C}$. First of all, we introduce the "Bloch" Hamiltonian $\mathcal{H}(k)$ and rewrite it in terms of β as $\mathcal{H}(\beta)$. Then the eigenvalue equation $\det[\mathcal{H}(\beta) - E] = 0$ is an algebraic equation for β, and let $2M$ be the degree of the equation. The main result is that when the eigenvalue equation has solutions β_i $(i = 1, \cdots, 2M)$ with $|\beta_1| \leq |\beta_2| \leq \cdots \leq |\beta_{2M-1}| \leq |\beta_{2M}|$, C_β is given by the trajectory of β_M and β_{M+1} under a condition $|\beta_M| = |\beta_{M+1}|$. It is obtained as the condition to construct continuum bands, which reproduce band structure for a large crystal with open boundaries. We note that in Hermitian systems, this condition reduces to $C_\beta : |\beta| = 1$, meaning that k becomes real. In the previous works, systems with $M = 1$ have been studied in general cases[83] and in limited cases[95].

A byproduct of our theory is that one can prove the bulk-edge correspondence. The bulk-edge correspondence has been discussed, but in most cases, it has not been shown rigorously but by observation on some particular cases, together with an analogy to Hermitian systems. It in fact shows that the bulk-edge correspondence for the real Bloch wave vector cannot be true in non-Hermitian systems. In this paper, we show the bulk-edge correspondence in the non-Hermitian SSH model with the generalized Brillouin zone, and discuss the relationship between a topological invariant in the bulk and existence of the edge states.

We start with a 1D tight-binding model, with its Hamiltonian given by

$$H = \sum_n \sum_{i=-N}^{N} \sum_{\mu,\nu=1}^{q} t_{i,\mu\nu} c_{n+i,\mu}^\dagger c_{n,\nu}, \tag{1}$$

where N represents the range of the hopping and q represents the degrees of freedom per unit cell. This Hamiltonian can be non-Hermitian, meaning that $t_{i,\mu\nu}$ is not necessarily equal to $t_{-i,\nu\mu}^*$. Then one can write the real-space eigen-equation as $H|\psi\rangle = E|\psi\rangle$, where the eigenvector is written as $|\psi\rangle = (\cdots, \psi_{1,1}, \cdots, \psi_{1,q}, \psi_{2,1}, \cdots, \psi_{2,q}, \cdots)^{\mathrm{T}}$ in an open chain. Thanks to the spatial periodicity, one can write the eigenvector as a linear combination:

$$\psi_{n,\mu} = \sum_j \phi_{n,\mu}^{(j)},\ \phi_{n,\mu}^{(j)} = (\beta_j)^n \phi_\mu^{(j)},\ (\mu = 1, \cdots, q). \tag{2}$$

By imposing that $\phi_{n,\mu}^{(j)}$ is an eigenstate, one can obtain the eigenvalue equation (for example, see Eq. (7)) for $\beta = \beta_j$ as

$$\det[\mathcal{H}(\beta) - E] = 0. \tag{3}$$

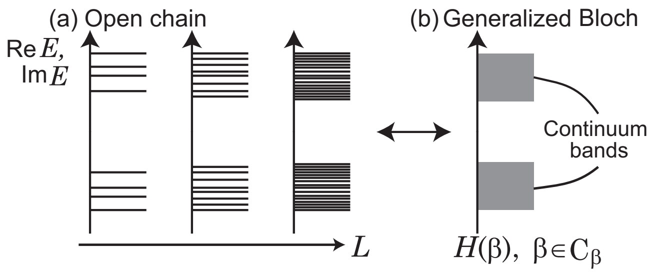

FIG. 1. Schematic figure of the band structure (a) in a finite open chain with various system sizes L, and (b) of the generalized Bloch Hamiltonian. The vertical axis represents the distribution of the complex energy E.

Here this eigenvalue equation is an algebraic equation for β with an even degree $2M$ in general cases[96].

One can see from Eq. (2) that β corresponds to the Bloch wave number $k \in \mathbb{R}$ via $\beta = \mathrm{e}^{ik}$ in Hermitian systems. The bulk-band structure for reality of k reproduces the band structure of a long open chain. When extending this idea to non-Hermitian systems, we should choose the values of β such that the bands of the Hamiltonian $\mathcal{H}(\beta)$ reproduce those of a long open chain (Fig. 1). The levels are discrete in a finite open chain, and as the system size becomes larger, the levels become dense and asymptotically form continuum bands (Fig. 1). Therefore, in order to find the generalized Brillouin zone C_β, one should consider asymptotic behavior of level distributions in an open chain in the limit of a large system size. In Hermitian systems, $|\beta|$ is equal to unity, meaning that the eigenstates extend over the bulk. On the other hand, in non-Hermitian systems, $|\beta|$ is not necessarily unity, and these states may be localized at an either end of the chain. Therefore these bands cannot be called bulk bands, but should be called continuum bands. These states are incompatible with the periodic boundaries. The continuum bands are formed by changing β continuously along C_β as we show later.

We find how to determine the generalized Brillouin zone C_β, which determines the continuum bands. Here we number the solutions β_i $(i = 1, \cdots, 2M)$ of Eq. (3) so as to satisfy $|\beta_1| \leq |\beta_2| \leq \cdots \leq |\beta_{2M-1}| \leq |\beta_{2M}|$. We find that the condition to get the continuum bands can be written as

$$|\beta_M| = |\beta_{M+1}|, \tag{4}$$

and the trajectory of β_M and β_{M+1} gives C_β. In Hermitian systems, we can prove that Eq. (4) becomes $|\beta_M| = |\beta_{M+1}| = 1$[96], and C_β is a unit circle $|\beta| = 1$. When $M = 1$, this condition physically corresponds to a condition for formation of a standing wave in an open chain as proposed in Ref. 83. We discuss this point in Sec. SI in Supplemental Material[96].

To get Eq. (4), we focus on boundary conditions in an open chain. Here we outline the discussion to show Eq. (4), and give the detailed discussion in Secs. SII and SIII in Supplemental Material[96]. We impose the wave

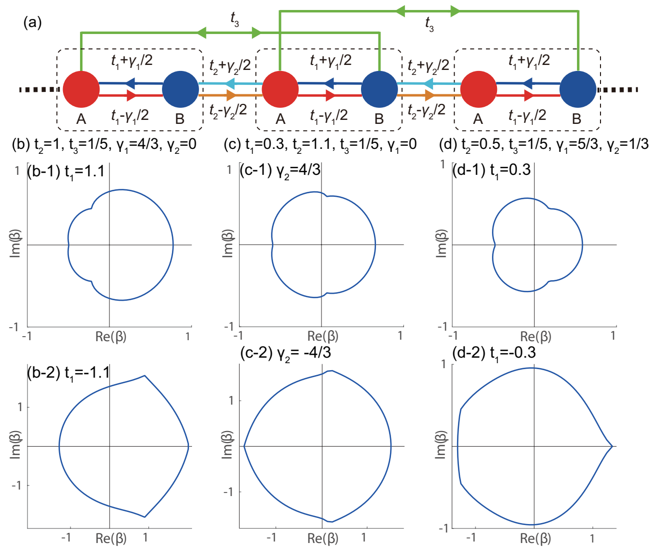

FIG. 2. (a) Non-Hermitian SSH model. The dotted boxes indicate the unit cell. (b)-(d) Generalized Brillouin zone C_β of this model. The values of the parameters are (b) $t_2 = 1, t_3 = 1/5, \gamma_1 = 4/3$, and $\gamma_2 = 0$; (b-1): $t_1 = 1.1$ and (b-2): $t_1 = -1.1$, (c) $t_1 = 0.3, t_2 = 1.1, t_3 = 1/5$, and $\gamma_1 = 0$; (c-1): $\gamma_2 = 4/3$ and (c-2): $\gamma_2 = -4/3$, and (d) $t_2 = 0.5, t_3 = 1/5, \gamma_1 = 5/3$, and $\gamma_2 = 1/3$; (d-1): $t_1 = 0.3$ and (d-2): $t_1 = -0.3$.

function Eq. (2) to represent an eigenstate. Apart from the positions near the two ends, it leads to the eigenvalue equation Eq. (3). The boundary conditions give another constraint onto the values of β_i $(i = 1, \cdots, 2M)$ in a form of an algebraic equation. We now suppose the system size L to be quite large, and consider a condition to achieve a densely distributed levels (Fig. 1). The equation consists of terms of the form $(\beta_{i_1}\beta_{i_2}\cdots\beta_{i_M})^L$. When $|\beta_M| \neq |\beta_{M+1}|$, there is only one leading term proportional to $(\beta_{M+1}\cdots\beta_{2M})^L$, which does not allow continuum bands. Only when $|\beta_M| = |\beta_{M+1}|$, there are two leading terms proportional to $(\beta_M\beta_{M+2}\cdots\beta_{2M})^L$ and to $(\beta_{M+1}\beta_{M+2}\cdots\beta_{2M})^L$. In such a case, the relative phase between β_M and β_{M+1} can be changed almost continuously for a large L, producing the continuum bands. We note that our condition Eq. (4) is independent of any boundary conditions. In Ref. 83, it was proposed that the continuum bands require $|\beta_i| = |\beta_j|$. Nonetheless it is not sufficient; except for the case $|\beta_M| = |\beta_{M+1}|$, it does not allow the continuum bands.

We apply Eq. (4) to the non-Hermitian SSH model as shown in Fig. 2 (a). It is given by

$$\begin{aligned} H = \sum_n \Big[& \left(t_1 + \frac{\gamma_1}{2}\right) c^\dagger_{n,\mathrm{A}} c_{n,\mathrm{B}} + \left(t_1 - \frac{\gamma_1}{2}\right) c^\dagger_{n,\mathrm{B}} c_{n,\mathrm{A}} \\ & + \left(t_2 + \frac{\gamma_2}{2}\right) c^\dagger_{n,\mathrm{B}} c_{n+1,\mathrm{A}} + \left(t_2 - \frac{\gamma_2}{2}\right) c^\dagger_{n+1,\mathrm{A}} c_{n,\mathrm{B}} \\ & + t_3 \left(c^\dagger_{n,\mathrm{A}} c_{n+1,\mathrm{B}} + c^\dagger_{n+1,\mathrm{B}} c_{n,\mathrm{A}} \right) \Big], \end{aligned} \tag{5}$$

where t_1, t_2, t_3, γ_1, and γ_2 are real. The generalized Bloch

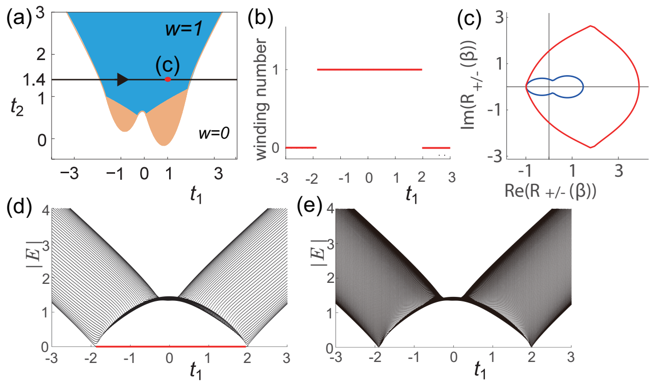

FIG. 3. (Color online) Phase diagram and bulk-edge correspondence with $t_3 = 1/5, \gamma_1 = 5/3$, and $\gamma_2 = 1/3$. (a) Phase diagram on the t_1-t_2 plane. The blue region represents that the winding number is 1, and the orange region represents that the system has exceptional points. Along the black arrow in (a) with $t_2 = 1.4$, we show the results for (b) the winding number, (d) energy bands in a finite open chain, and (e) the continuum bands from the generalized Brillouin zone C_β. The edge states are shown in red in (d). (c) shows ℓ_+ (red) and ℓ_- (blue) on the $\boldsymbol{R}$ plane with $t_1 = 1$ and $t_2 = 1.4$.

Hamiltonian $\mathcal{H}(\beta)$ can be obtained by a replacement $e^{ik} \to \beta$, similarly to Hermitian systems, as $\mathcal{H}(\beta) = R_+(\beta)\sigma_+ + R_-(\beta)\sigma_-$, where $\sigma_\pm = (\sigma_x \pm i\sigma_y)/2$, and $R_\pm(\beta)$ are given by

$$R_+(\beta) = \left(t_2 - \frac{\gamma_2}{2}\right)\beta^{-1} + \left(t_1 + \frac{\gamma_1}{2}\right) + t_3\beta,$$
$$R_-(\beta) = t_3\beta^{-1} + \left(t_1 - \frac{\gamma_1}{2}\right) + \left(t_2 + \frac{\gamma_2}{2}\right)\beta. \quad (6)$$

Therefore the eigenvalue equation can be written as

$$R_+(\beta)R_-(\beta) = E^2, \quad (7)$$

which is a quartic equation for β, i.e. $M = 2$, having four solutions β_i $(i = 1, \cdots, 4)$ satisfying $|\beta_1| \le |\beta_2| \le |\beta_3| \le |\beta_4|$. Then Eq. (4) is given by $|\beta_2| = |\beta_3|$[96].

The trajectory of β_2 and β_3 satisfying the condition $|\beta_2| = |\beta_3|$ determines the generalized Brillouin zone C_β, and it is shown in Figs. 2 (b)-(d) for various values of the parameters. It always forms a loop enclosing the origin on the complex plane. Nonetheless we do not have a rigorous proof that C_β is always a single loop encircling the origin. We find some features of C_β. Firstly our result does not depend on whether $|\beta|$ is larger or smaller than unity, as opposed to the suggestions in the previous works[57,83]; in Fig. 2 (d-2), $|\beta|$ takes both the values more than and less than 1. Secondly C_β can be a unit circle even for non-Hermitian cases, for example, when $t_1 = t_3 = \gamma_2 = 0$. Finally C_β can have cusps, corresponding to the cases with three solutions share the same absolute value[96].

We calculate the winding number w for the Hamiltonian $\mathcal{H}(\beta)$. Thanks to the chiral symmetry, w can be defined as[96]

$$w = -\frac{w_+ - w_-}{2}, \; w_\pm = \frac{1}{2\pi}\left[\arg R_\pm(\beta)\right]_{C_\beta}, \quad (8)$$

where $[\arg R_\pm(\beta)]_{C_\beta}$ means the change of the phase of $R_\pm(\beta)$ as β goes along the generalized Brillouin zone C_β in the counterclockwise way. It was proposed that w corresponds to the presence or absence of the topological edge states[83].

We show how the gap closes in our model. It closes when $E = 0$, i.e. $R_+(\beta) = 0$ or $R_-(\beta) = 0$. Let $\beta = \beta_i^a$ $(i = 1, 2, \; a = +, -)$ denote the solutions of the equation $R_a(\beta) = 0$ with $|\beta_1^a| \le |\beta_2^a|$. When $E = 0$ is in the continuum bands, Eq. (4) should be satisfied for the four solutions $\beta_i^\pm$ $(i = 1, 2)$. It can be classified into two cases, (a) $|\beta_1^a| \le |\beta_2^a| = \left|\beta_1^{-a}\right| \le \left|\beta_2^{-a}\right|$ $(a = +, -)$, and (b) $|\beta_1^a| \le \left|\beta_1^{-a}\right| = \left|\beta_2^{-a}\right| \le |\beta_2^a|$ $(a = +, -)$. In the case (a), as one changes one parameter, the gap closes at $E = 0$ and w_+ and $-w_-$ change by one at the same time, giving rise to the change of the winding number by unity. On the other hand, in the case (b), only one of the two coefficients $R_\pm(\beta)$ becomes zero, and it represents an exceptional point.

We obtain the phase diagram on the t_1-t_2 plane in Fig. 3 (a) and one on the γ_1-γ_2 plane in Fig. 4 (a). In these phase diagrams, the winding number w is 1 in the blue region. By definition, w changes only when $R_\pm(\beta) = 0$ on the generalized Brillouin zone C_β, and the gap closes. The energy bands in a finite open chain calculated along the black arrow in Fig. 3 (a) are shown in Fig. 3 (d), and one can confirm that the edge states appear in the region where $w = 1$. In addition, the continuum bands using C_β (Fig. 3 (e)) agree with these energy bands. In Fig. 4 (b), we give the energy bands calculated along the green arrow in Fig. 4 (a), and the edge states appear similarly to Fig. 3 (d). On the other hand, the system has the exceptional points in the orange region. The phase with the exceptional points extends over a finite region[96].

We discuss the bulk-edge correspondence in our model. The loops $\ell_\pm$ drawn by $R_\pm(\beta)$ on the $\boldsymbol{R}$ plane are shown in Fig. 3 (c) and Figs. 4 (c) and (d) for certain values of the parameters. Both in Fig. 3 (c) and in Fig. 4 (c), the system has the winding number $w = 1$ since both ℓ_+ and ℓ_- surround the origin $\mathcal{O}$, leading to $w_+ = -1$ and $w_- = 1$. In Fig. 4 (a), one can continuously change the values of the parameters to the Hermitian limit, $\gamma_1, \gamma_2 \to 0$, while keeping the gap open and $w = 1$ remain. The same is true for Fig. 3 (a). Therefore, by following the proof in Hermitian cases[97], one can prove the bulk-edge correspondence even for the non-Hermitian cases, and existence of zero-energy states is derived[96]. On the other hand, ℓ_- passes $\mathcal{O}$ as shown in Fig. 4 (d), where the system has the exceptional points. We note that the winding number is not well-defined in this case.

In summary, we establish a generalized Bloch band theory in 1D tight-binding systems, and obtain the condition for the continuum bands. We show the way to construct the generalized Brillouin zone C_β, which is fundamental for obtaining the continuum bands. Here the Bloch wave number k takes complex values in non-Hermitian systems. Our conclusion, $|\beta_M| = |\beta_{M+1}|$, is physically

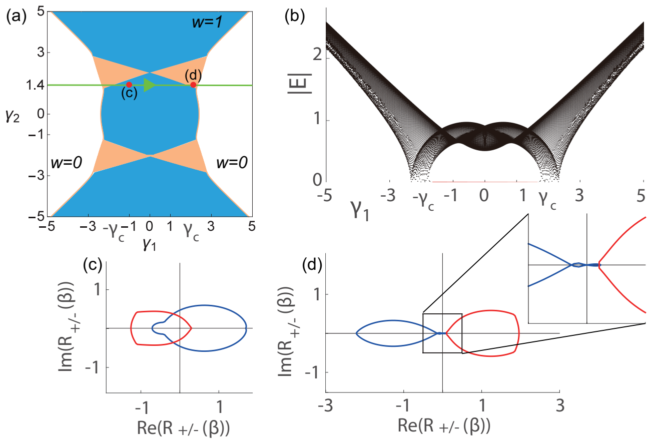

FIG. 4. Phase diagram and bulk-edge correspondence with $t_1 = 0, t_2 = 1$, and $t_3 = 1/5$. (a) Phase diagram on the γ_1-γ_2 plane. The blue region represents that the winding number is 1, and the orange region represents that the system has exceptional points. (b) Energy bands calculated along the green arrow in (a) with $\gamma_2 = 1.4$. Note that $\gamma_c \simeq 1.89$. The edge states are shown in red. (c)-(d) Loops ℓ_+ (red) and ℓ_- (blue) on the $\boldsymbol{R}$ plane. The values of the parameters are (c) $\gamma_1 = -1$ and $\gamma_2 = 1.4$, and (d) $\gamma_1 = 2.1$ and $\gamma_2 = 1.4$. Note that ℓ_- passes the origin in (d), which corresponds to exceptional points.

reasonable in several aspects. First it is independent of any boundary conditions. Thus, for a long open chain, irrespective of any boundary conditions, the spectrum asymptotically approaches the same continuum bands calculated from C_β[96]. Second it reproduces the known result in the Hermitian limit, i.e. $|\beta| = 1$. Third the form of the condition is invariant under a replacement $\beta \to 1/\beta$. Suppose the numbering of the sites is reversed by putting $n' = L+1-n$ for the site index $n (= 1, \cdots, L)$; then β becomes $\beta' = 1/\beta$, but the form of the condition is invariant: $|\beta'_M| = |\beta'_{M+1}|$.

Through this definition of the continuum bands, one can show the bulk-edge correspondence without ambiguity by defining the winding number w from the generalized Brillouin zone in 1D systems with chiral symmetry. Indeed we showed that the zero-energy states appear in the non-Hermitian SSH model when w takes non-zero values, and also revealed that these states correspond to topological edge states. It is left for future works how to calculate the continuum bands for systems with other symmetries.

The construction of the generalized Brillouin zone can be extended to higher dimensions as well. In two-dimensional (2D) systems, we introduce the two parameters $\beta^x \left(= \mathrm{e}^{ik_x}\right)$ and $\beta^y \left(= \mathrm{e}^{ik_y}\right)$. Then the eigenvalue equation $\det\left[\mathcal{H}\left(\beta^x, \beta^y\right) - E\right] = 0$, where $\mathcal{H}\left(\beta^x, \beta^y\right)$ is a 2D generalized Bloch Hamiltonian, is an algebraic equation for β^x and β^y. If we fix β^y (β^x), this system can be regarded as a 1D system, and the criterion is given by $\left|\beta^x_{M_x}\right| = \left|\beta^x_{M_x+1}\right|$ $\left(\left|\beta^y_{M_y}\right| = \left|\beta^y_{M_y+1}\right|\right)$, where $2M_x$ $(2M_y)$ is the degree of the eigenvalue equation for β^x (β^y). Thus we can get the conditions for the continuum bands. Nevertheless it is still an open question how to determine the generalized Brillouin zone in higher dimensions.

We also apply our theory to the tight-binding model proposed in Ref. 74, and show that the Bloch wave number k has a nonzero imaginary part, and the bulk-edge correspondence can be established with $k \in \mathbb{C}$[96]. We conclude that some previous works on the bulk-edge correspondence using reality of the Bloch wave vector require further investigations.

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