Editors' Suggestion

Correspondence between Winding Numbers and Skin Modes in Non-Hermitian Systems

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We establish exact relations between the winding of "energy" (eigenvalue of Hamiltonian) on the complex plane as momentum traverses the Brillouin zone with periodic boundary condition, and the presence of "skin modes" with open boundary conditions in non-Hermitian systems. We show that the nonzero winding with respect to any complex reference energy leads to the presence of skin modes, and vice versa. We also show that both the nonzero winding and the presence of skin modes share the common physical origin that is the nonvanishing current through the system.

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Introduction.—Some systems that are coupled to energy or particle sources or drains, or driven by external fields, can be effectively modeled Hamiltonians having non-Hermitian terms [1–9]. For example, one may add a diagonal imaginary part in a band Hamiltonian for electrons to represent the effect of finite quasiparticle lifetime [10–13]. One may also introduce an imaginary part to the dielectric constant in Maxwell equations to represent metallic conductivity in a photonic crystal [14–20]. As non-Hermitian operators in general have complex eigenvalues, the eigenfunctions of Schrödinger equations are no longer static, but decay or increase exponentially in amplitude with time [21,22].

A topic in recent condensed-matter research is the study of topological properties in band structures, which are generally given by the wave functions, *not* the energy, of all occupied bands (or more generally, a group of bands capped from above and below by finite energy gaps) [23–27]. The topological band theory has been extended to non-Hermitian systems and further developed in recent years [28–31]. In non-Hermitian systems, obviously, one immediately identifies a different type of topological numbers in bands, given by the phase winding of the "energy" (eigenvalue of Hamiltonian), *not* the wave functions, in the Brillouin zone (BZ) [32]. This *winding number*, together with several closely related winding numbers if other symmetries are present, give topological classification that is richer than that of their Hermitian counterparts [22,30,33–36]. Besides winding in energy in the complex plane, another unique phenomenon recently proposed in non-Hermitian systems is the non-Hermitian skin effect in open-boundary systems [36–54], which has also been verified experimentally [55–58], and a simple example of skin modes can be seen in the Supplemental Material, Sec. I [59]. A typical spectrum of an open Hermitian system consists of a large number of bulk states, and, if at all, a small number of edge states, and as the system increases in size L, the numbers of the bulk and of the edge states increase as L^d and L^{d-n}, respectively, where d is the dimension and $0 < n \leq d$. However, in certain non-Hermitian systems, a finite fraction, if not all, of eigenstates are concentrated on one of the edges. These non-Hermitian skin modes decay exponentially away from the edges just like edge states, but their number scales as the volume (L^d), rather than the area, of the system [62].

In this Letter, we show an exact relation between the new quantum number, i.e., the winding number of energy with periodic boundary, and the existence of skin modes with open boundary, for any one-band model in one dimension. To do this, we first extend the one-band Hamiltonian with finite-range hopping $H(k)$ to a holomorphic function $H(z) = P_{n+m}(z)/z^m$ $(n, m > 0)$ [63], where $P_{n+m}(z)$ is a $(n+m)$ polynomial, and the Brillouin zone maps to unit circle $|z| = 1$ (or $z = e^{ik}$). The image of the unit circle under $H(z)$ is the spectrum of the system with periodic boundary, and generally, it forms a loop on the complex plane, $\mathcal{L}_{\rm BZ} \in \mathbb{C}$. Then we show that as long as $\mathcal{L}_{\rm BZ}$ has finite interior, or roughly speaking encloses a finite area, skin modes appear as eigenstates with open boundary conditions; but when $\mathcal{L}_{\rm BZ}$ collapses into a curve having no interior on the complex plane, the skin modes disappear. In other words, skin modes with open boundary appear if and only if there is $E_b \in \mathbb{C}$ with respect to which $\mathcal{L}_{\rm BZ}$ has nonzero winding. Finally, we show that the winding of the periodic boundary spectrum, and hence the presence of skin modes with open boundary, are related to the total persistent current of the system. We prove that if the current vanishes for all possible state distribution functions

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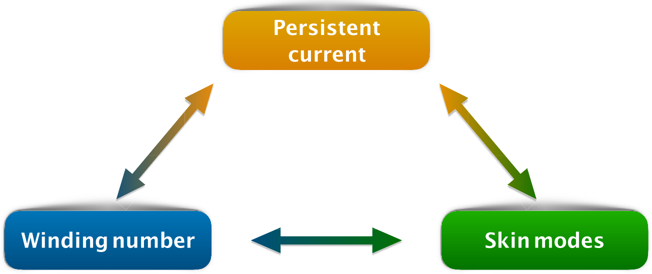

FIG. 1. The reciprocal relations among the three phenomena unique to non-Hermitian systems: the nonvanishing persistent current, nonzero winding number of energy, and the presence of skin modes. The validity of any one is the sufficient and necessary condition for the validity of the other two.

$n(H, H^*)$, the winding and the skin modes also vanish, and vice versa. The relations we establish among nonzero winding, presence of skin modes, and nonvanishing current are summarized in Fig. 1. Some of the results are extended to 1D models with multiple bands.

Hamiltonian as a holomorphic function.—We start with an arbitrary one-band tight-binding Hamiltonian in one dimension, only requiring that hoppings between i and j sites only exist within a finite range $-m \leq i - j \leq n$.

$$H = \sum_{i,j} t_{i-j} |i\rangle\langle j| = \sum_{k \in \mathrm{BZ}} H(k) |k\rangle\langle k|, \tag{1}$$

where $H(k) = \sum_{r=-m,\ldots,n} t_r (e^{ik})^r$ is the Fourier transformed t_r (t_0 being understood as the on-site potential). For periodic boundary condition, we have $0 \leq k < 2\pi$, and e^{ik} moves along the unit circle on the complex plane. For future purposes, we define $z \coloneqq e^{ik}$, and consider z as a general point on the complex plane. Therefore for each Hamiltonian $H(k)$, we now have a holomorphic function

$$H(z) = t_{-m} z^{-m} + \cdots + t_n z^n = \frac{P_{m+n}(z)}{z^m}, \tag{2}$$

where $P_{m+n}(z)$ is a polynomial of order $m+n$. $H(z)$ has one composite pole at $z = 0$, the order of which is m, and has $m+n$ zeros, i.e., the zeros of the $(m+n)$ polynomial. Along any oriented loop $\mathcal{C}$ and any given reference point $E_b \in \mathbb{C}$, one can define the winding number of $H(z)$

$$w_{\mathcal{C},E_b} \coloneqq \frac{1}{2\pi} \oint_{\mathcal{C}} \frac{d}{dz} \arg[H(z) - E_b] dz. \tag{3}$$

Specially, for $\mathcal{C} = \mathrm{BZ}$, $w_{\mathcal{C},E_b}$ is the winding of the phase of $H(z) - E_b$ along BZ, considered as a new topological number unique to non-Hermitian systems [22,30,32–36,64]. The Cauchy principle relates the winding number of any complex function $f(z)$ to the total number of zeros and poles enclosed in $\mathcal{C}$, that is,

$$w_{\mathcal{C},E_b} = N_{\mathrm{zeros}} - N_{\mathrm{poles}}, \tag{4}$$

where $N_{\mathrm{zeros,\,poles}}$ is the counting of zeros (poles) weighted by respective orders. See Figs. 2(a),(b) for the pole, the zeros, and the winding of $\mathcal{L}_{\mathrm{BZ}}$ for a specific Hamiltonian. In fact, we always have $N_{\mathrm{poles}} = m$, so that the winding number is determined by the number of zeros of $P_{m+n}(z) - z^m E_b$ that lie within the unit circle. As we will see later, the advantage of extending the Hamiltonian into a holomorphic function lies in exactly this relation between the winding numbers and the zeros.

Generalized Brillouin zone.—In Refs. [36,38,42], it is shown that the energy spectrum of certain non-Hermitian systems with open boundary may deviate drastically from that with periodic boundary, due to the presence of skin modes [38–40]. Furthermore, in Refs. [38,65], the authors introduce a new concept of the generalized Brillouin zone to signify the difference between the periodic and open boundary: instead of evaluating $H(z)$ along BZ, the open-boundary energy spectrum is recovered as one evaluates $H(z)$ on another closed loop called GBZ as L goes to infinity. The GBZ is determined by the equation

$$\mathrm{GBZ} \coloneqq \{z \| H_m^{-1}[H(z)] | = |H_{m+1}^{-1}[H(z)]|\}, \tag{5}$$

where $H_i^{-1}(E)$'s satisfying $|H_i^{-1}(E)| \leq |H_{i+1}^{-1}(E)|$ are the $m+n$ branches of the inverse function of $H(z)$. (In Ref. [65], $m = n$ is assumed, and we extend the results to $m \neq n$ cases in the Supplemental Material, Sec. II [59].) We emphasize that using GBZ, one can compute the open boundary spectrum of systems of large or infinite size by solving some algebraic equations such as Eq. (5), a process we sketch using the following steps. To begin with, one finds the inverse functions of $H(z)$, and orders them in ascending amplitude, thus obtaining $H_i^{-1}(E)$, where $i = 1, \ldots, m+n$ because the $P_{m+n}(z) - Ez^m$ is an order $m+n$ polynomial of z. Then, as there are two variables $[\mathrm{Re}(E), \mathrm{Im}(E)]$ in Eq. (5), by codimension counting its solution on the complex plane forms one or several close loops, which are nothing but the open boundary energy spectrum. Finally, one substitutes these solutions back into $H_m^{-1}(E)$. It is noted that if we are only interested in the spectrum, we may stop at the second last step, but we need GBZ in order to articulate some of our key results.

With GBZ thus defined, we state our central result (for proof see the Supplemental Material, Sec. III [59]): GBZ is the closed curve in the complex plane that encloses the pole (at the origin) of order m and exactly m zeros of $P_{m+n}(z) - Ez^m$ for arbitrary $E \in \mathbb{C}$ [66]. This seemingly technical result has the following consequences. First, this means within GBZ the total number of zeros and poles (weighted by respective orders) cancels, so that the winding of $H(z) - E$ vanishes. Next, the arbitrariness of E ensures that GBZ is invariant under a shift of energy origin in the complex plane $H(z) \to H_z - E_b$. Combining these two points, we see that

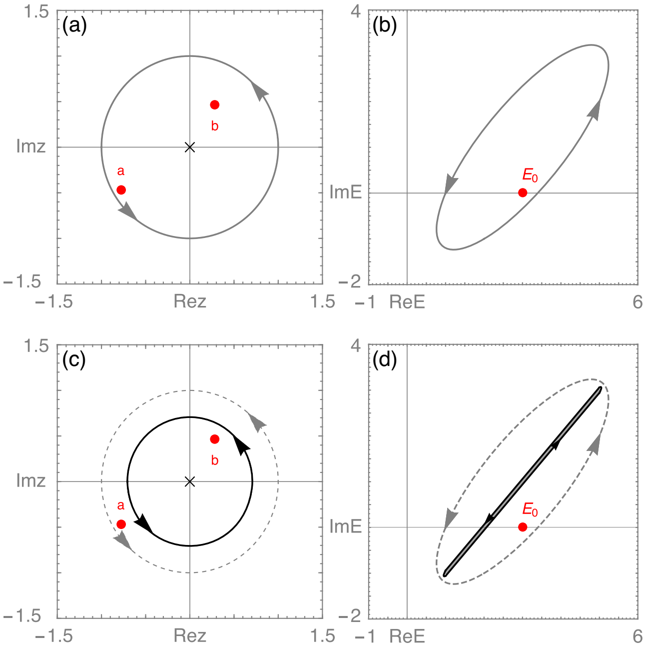

FIG. 2. We show the BZ (a) with periodic-boundary spectrum (b), and GBZ (c) with open boundary spectrum (d) for the model $H(z) = [2iz^2 + (3+i)z + 1]/z$, and the red dot $E_0 = H(z = a) = H(z = b) = 3$ is the reference energy with respect to which winding is defined. In (a),(c) the red dots represent the zeros of $H(z) - E_0 = 0$, and the cross denotes the pole. We remark that the orientation of GBZ in (c) is arbitrarily chosen.

the image of GBZ under $H(z)$ on the complex plane, denoted by $\mathcal{L}_{\rm GBZ}$, has zero winding with respect to any $E_b \in \mathbb{C}$, or symbolically,

$$w_{{\rm GBZ},E_b} = 0, \tag{6}$$

where the orientation of GBZ is defined in the Supplemental Material, Sec. III [59]. Therefore, we finally see that the open-boundary spectrum of $H(z)$ cannot be a circle or eclipse like the periodic-boundary counterpart, and it cannot even form a loop enclosing any finite area, because in that case one can choose E_b inside that area so that the winding of $\mathcal{L}_{\rm GBZ}$ with respect to E_b is nonzero. The only possibility is that $\mathcal{L}_{\rm GBZ}$ *collapses* into an arc as shown in Fig. 2(d). In this specific example ($m = n = 1$ and see caption for parameters), we plot the GBZ in Fig. 2(c) and $\mathcal{L}_{\rm GBZ}$ in Fig. 2(d) as z moves counterclockwise along the GBZ. We see that while GBZ is more or less a circle, its image $\mathcal{L}_{\rm GBZ}$ keeps "back stepping" itself: except for a few turning and branching points, any point in $\mathcal{L}_{\rm GBZ}$ has two or an even number of preimages in the GBZ, so that the end result looks like more connected segments of curves than a closed loop.

Skin modes and nonzero winding numbers.—GBZ not only gives the open boundary spectrum, but also yields information on the eigenstates with open boundary [38,65]. In fact, each point $z \in$ GBZ represents an eigenstate, the wave function of which is in the form $\langle s|\psi(z)\rangle \propto |z|^s$, where $s = 1, \ldots, L$ labels the sites. When $|z| > 1$ ($|z| < 1$), the wave function is concentrated near the ($s = 1$) edge [($s = L$) edge] and exponentially decays with distance from the edge [see Figs. 3(a3),(b3),(c3) for examples]. Therefore, any part of the GBZ that lies within (without) the unit circle corresponds to a set of skin modes. In extreme cases, when the entire GBZ is inside (outside) the unit circle, all eigenstates are skin modes on the left (right) side of the chain. In short, any deviation of GBZ from BZ signifies the existence of skin modes.

For a given $H(z)$, if $w_{{\rm BZ},E_b} \neq 0$, then from Eq. (6) we have $w_{{\rm GBZ},E_b} = 0$, hence GBZ must deviate from the unit circle, that is, skin modes must exist with open boundary. Let us now try to prove the inverse statement: if GBZ and BZ differ from each other, then one can always find a $E_b \in \mathbb{C}$ such that $w_{{\rm BZ},E_b} \neq 0$. GBZ and BZ may differ from each other in three typical ways: (i) as in Fig. 3(a1), GBZ contains the unit circle, and we define U as the region

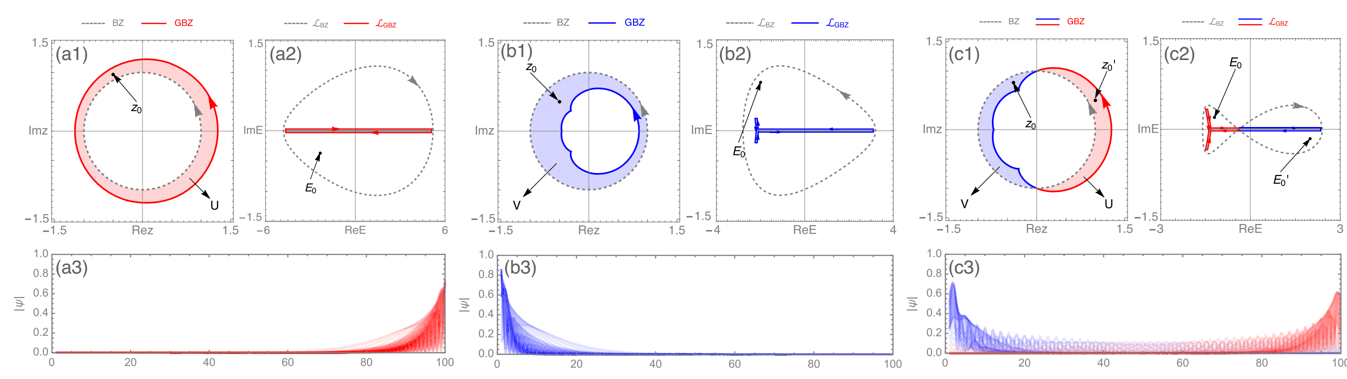

FIG. 3. BZ and GBZ, periodic- and open-boundary spectra, and all normalized eigenfunctions for open boundary are plotted for $H(z) = z^{-2}/5 + 3z^{-1} + 2z$ in (a1)–(a3), $H(z) = z^{-2}/5 + z^{-1} + 2z$ in (b1)–(b3), and $H(z) = 2z^{-2}/5 + z^{-1} + z$ in (c1)–(c3). The regions inside BZ (GBZ) and outside GBZ (BZ) are colored in blue (red), and the eigenfunctions corresponding to points on GBZ outside (inside) BZ are plotted as red (blue) curves. z_0, z_0' are randomly chosen points in the red and the blue regions, respectively, and $E_0 = H(z_0)$, $E_0' = H(z_0')$.

inside GBZ but outside BZ (colored in red); (ii) as in Fig. 3(b1), GBZ is contained in the unit circle, and we define V as the region outside GBZ but inside BZ (colored in blue); (iii) as in Fig. 3(c1), one part of GBZ is outside and another part inside the unit circle. For case (i), pick $z_0 \in U$ and $E_0 = H(z_0)$. z_0 is then a zero of $H(z_0) - E_0$, and from Eq. (6), we know there are exactly m zeros inside GBZ, so inside BZ there are at most $m-1$ zeros, and from Eq. (4) we have $w_{\mathrm{BZ},E_0} < -1 \neq 0$ [see example in Fig. 3(a2)]. For case (ii), pick $z_0' \in V$ and $E_0' = H(z_0')$, then use similar arguments to see $w_{\mathrm{BZ},E_0'} > 1 \neq 0$ [see example in Fig. 3(b2)]. We postpone the proof for case (iii) to the Supplemental Material, Sec. IV [59], but mention here that for $z_0 \in U$ and $z_0' \in V$, the periodic-boundary spectrum $\mathcal{L}_{\mathrm{BZ}}$, taking the shape of a fish [see Fig. 3(c2)], has opposite windings with respect to E_0 and E_0'.

Winding numbers, skin modes, and persistent current.—From the above results, we see that if and only if $\mathcal{L}_{\mathrm{BZ}}$ does not enclose any $E_b \in \mathbb{C}$, then the skin modes do not exist. When this is the case, $\mathcal{L}_{\mathrm{BZ}}$ always back steps itself just like $\mathcal{L}_{\mathrm{GBZ}}$, or more precisely, along $\mathcal{L}_{\mathrm{BZ}}$, for any small segment δH centered at some E, there must be another segment $-\delta H$ centered at exactly the same E. What is the physical meaning of this condition? We show that this is equivalent to the absence of total persistent current with periodic boundary. To define the current, we assume that the particles have some charge (taken to be unity), so the total persistent current can be derived as $J = \sum_k n_k v_k = \sum_k n_k H'(k) dk$, where n_k is some distribution function [67]. Now we make a general physical assumption that n_k only depends on the energy of the state, that is $n_k = n[H(k), H^*(k)]$, but does not depend on k explicitly. [Here n depends on both the real and the imaginary parts of $H(k)$, so is unnecessarily holomorphic.] For example, the Bose distribution $n_k = (e^{\mathrm{Re}[H(k)]/k_B T} - 1)^{-1}$ satisfies such a condition. When the curve $\mathcal{L}_{\mathrm{BZ}}$ has no interior, we have

$$J = \int_0^{2\pi} n(H, H^*) \frac{dH(k)}{dk} dk = \oint_{\mathcal{L}_{\mathrm{BZ}}} n(H, H^*) dH = 0, \quad (7)$$

that is, the total persistent current vanishes. In the Supplemental Material, Sec. V [59], we prove the inverse statement that if there is any $E_b \in \mathbb{C}$ with respect to which $H(z)$ has nonzero winding, then one can always find some $n(H, H^*) \neq 0$ such that $J \neq 0$. This equivalence is intuitively understood: if a persistent current is going around a ring, then as one cuts open the ring, the charge starts concentrating on one end of the open chain. This persistent current is a linear response and vanish for any Hermitian system, which is proved in the Supplemental Material, Sec. VI [59].

Discussion and conclusion.—So far we have established the reciprocal relations shown in Fig. 1 for the one-band model in one dimension. Some of the results may be extended to the cases of more bands and/or higher dimensions. For example, in d dimension, one should consider a multivariable holomorphic function $H(z_1, z_2, \ldots, z_d): \mathbb{C}^d \to \mathbb{C}$, where $z_j \coloneqq e^{ik_j}$, and the spectrum of $H(z_1, \ldots, z_d)$ is in general a continuum on the complex plane. Are there skin modes when we have open boundary along $0 < l \leq d$ directions, but periodic boundary along the other $d - l$ directions? We have two conjectures for two extreme cases: (i) if $l = d$, that is, if all directions are open, skin modes vanish if and only if each component persistent current vanishes for arbitrary $n(H, H^*)$; and (ii) if $l = 1$, that is, if only one direction is open, the skin modes vanish if and only if the entire spectra of $H(z_1, \ldots, z_d)$ collapse into a curve having no interior. The "only if" part of (i) and the "if" part of (ii) are only obvious, but the other parts seem not quite so.

Extension of the relation between the persistent current and the winding numbers in periodic boundary to multiple-band systems is straightforward. Now $H_{ab}(z)$ becomes a matrix function of $z \coloneqq e^{ik}$, where $a, b = 1, \ldots, n$ label the orbitals. The persistent current in this case becomes $J = \mathrm{Tr}(\hat{\rho}\hat{J}) = \sum_{i=1,\ldots,n} J_i$, where

$$J_i = \int_0^{2\pi} n(E_i, E_i^*) \frac{dE_{i,k}}{dk} = \oint_{\mathcal{L}_{i,\mathrm{BZ}}} n(E_i, E_i^*) dE_i. \quad (8)$$

The operators $\hat{\rho}$ and $\hat{J}$ are steady-state density matrix operator and current operator, expressed as, respectively, $\hat{\rho} = \sum_{i,k} n(E_{i,k}, E_{i,k}^*) |i_k^R\rangle\langle i_k^L|$ and $\hat{J} = \sum_{k,a,b} dH_{ab}(k)/dk |a_k\rangle\langle b_k|$. More details of derivation can be found in the Supplemental Material, Sec. VI [59]. While $J_i = 0$ implies $J = 0$, $J = 0$ does *not* necessitate $J_i = 0$ for each i. In fact, one part of the trajectory of $E_i(k)$ may be back stepped by another part of the trajectory of $E_{j\neq i}(k)$ so that their contribution to J cancel out. Therefore, $J = 0$ is equivalent to the collapse of the spectrum, not of each individual band, but of all bands, into a curve that has no interior. In more precise terms, $J = 0$ for arbitrary $n(E, E^*)$ if and only if for any $E_b \in \mathbb{C}$ and $E_b \notin \mathcal{L}_{i,\mathrm{BZ}}$, the total winding number of all bands with respect to E_b vanishes, or symbolically

$$\frac{1}{2\pi i} \int_0^{2\pi} \frac{d \log \det[H(z) - E_b I_{n\times n}]}{dk} dk = 0. \quad (9)$$

When there are additional conserved charges in the Hamiltonian, for example, some spin component, we can simply replace the total current J with the component current for each conserved charge J_c. At this point, we do not know exactly how the nonzero persistent current or the winding numbers are related to the skin modes in multiband systems, but from physical intuition, we conjecture that $J \neq 0$ implies skin modes with open boundary, and vice versa.

In summary, we theoretically demonstrate that a one-dimensional non-Hermitian Hamiltonian with open boundary condition has a non-Hermitian skin effect as long as the complex energy spectrum of the same Hamiltonian under periodic boundary condition makes a loop having nonzero area in the complex plane. The vanishing non-Hermitian skin effect is also related to the vanishing persistent current for an arbitrary density matrix of a steady state.

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Note added.—Recently, the authors became aware of a closely related work [68].

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