Bulk-Boundary Correspondence for Non-Hermitian Hamiltonians via Green Functions

Heinrich-Gregor Zirnstein, Gil Refael, and Bernd Rosenow

Phys. Rev. Lett. **126**, 216407 — Published 28 May 2021

DOI: 10.1103/PhysRevLett.126.216407

Bulk-boundary correspondence for non-Hermitian Hamiltonians via Green functions

Heinrich-Gregor Zirnstein,[1] Gil Refael,[2] and Bernd Rosenow[1,3]

[1] *Institut für Theoretische Physik, Universität Leipzig, Brüderstrasse 16, 04103 Leipzig, Germany*
[2] *Institute of Quantum Information and Matter and Department of Physics, California Institute of Technology, Pasadena, CA 91125, USA*
[3] *Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel*

(Dated: July 16, 2020)

Genuinely non-Hermitian topological phases can be realized in open systems with sufficiently strong gain and loss; in such phases, the Hamiltonian cannot be deformed into a gapped Hermitian Hamiltonian without energy bands touching each other. Comparing Green functions for periodic and open boundary conditions we find that, in general, there is no correspondence between topological invariants computed for periodic boundary conditions, and boundary eigenstates observed for open boundary conditions. Instead, we find that the non-Hermitian winding number in one dimension signals a topological phase transition in the bulk: It implies spatial growth of the bulk Green function.

Topology has made a profound impact on the description and design of wave-like systems such as quantum mechanical electrons [1–5] or light interacting with matter [6–11]. The key idea is to group physical systems, each described by a gapped (insulating) Hamiltonian, into the same topological class if their Hamiltonians can be continuously deformed into each other without closing the energy gap. For Hermitian Hamiltonians, the *bulk-boundary correspondence* states that topological invariants for periodic boundary conditions predict the presence of boundary states for open boundary conditions [1, 12–16].

Recently, non-Hermitian Hamiltonians [17–21] have attracted much attention; they describe open systems with loss (dissipation) and gain (e.g. coherent amplification in a laser) [22, 23]. Extending topological methods to these systems may be particularly beneficial for the design of topological protected laser modes [24–26]. Moreover, *genuinely non-Hermitian Hamiltonians*, i.e. Hamiltonians that cannot be deformed to a Hermitian Hamiltonian without energy bands touching, have novel topological properties not found in Hermitian systems. They can be characterized by topological invariants different from those of Hermitian systems [27–38], but the extent of a bulk-boundary correspondence is, surprisingly, much less clear [39–50].

We consider systems in one dimensions, which are particularly interesting because not only the eigenvectors but also the eigenenergies can have a nontrivial winding number. In the case of a two-band model with chiral symmetry, the Bloch Hamiltonian is off-diagonal

$$H(k) = \begin{pmatrix} 0 & q_+(k) \\ q_-(k) & 0 \end{pmatrix}. \tag{1}$$

In a lattice model, the lattice spacing forces the momentum k to be periodic, and the $q_\pm(k)$ describe closed paths in the complex plane. For example, a non-Hermitian Su-Schrieffer-Heeger (SSH) model is given by $q_\pm(k) = (m-1) + e^{\pm(\gamma - ik)}$, and the paths are circles with different radii centered on the real axis. [51] The eigenvalues of the matrix $H(k)$ are distinct if neither path passes through the origin; in this case, we can assign to each path a winding number around the origin. These form the $\mathbb{Z}\times\mathbb{Z}$ topological invariant of a non-Hermitian Hamiltonian in symmetry class AIII [28]. Hermitian Hamiltonians are characterized by $q_+(k) = q_-(k)^*$, which forces both winding numbers to be opposites of each other; a single $\mathbb{Z}$-invariant remains [3, 52, 53]. Genuinely non-Hermitian phases appear whenever the two winding numbers are no longer opposites of each other [28, 33]. In this case, the *non-Hermitian winding number*, which is the winding number of the determinant $\det(H(k))$, is nonzero.

Is there a bulk-boundary correspondence for the non-Hermitian winding number? To answer this, we focus on response (Green) functions, which describe experimental observables in a scattering setup. We find that the bulk-boundary correspondence breaks down once the non-Hermitian winding number takes a non-trivial value: When the winding number changes from zero, the bulk response starts exhibiting exponential *growth* in space, and since periodic systems cannot accommodate such spatial growth, they do not reflect the properties of systems with open boundaries. In this Letter, we focus on the specific example of non-Hermitian Dirac fermions to discuss the above physics, while a general proof is contained in the companion paper Ref. [54]. Green functions are more robust objects than eigenstates, because the latter are very sensitive to boundary conditions: wave functions can become localized in the presence of an open boundary, a phenomenon referred to as non-Hermitian skin effect [39, 41, 55–64]. This skin effect can be observable already for arbitrarily small non-Hermiticity, whereas an exponential growth of the bulk

Green function occurs only above a critical strength of non-Hermiticity. In a semi-infinite system with only one boundary on the other hand, right-eigenfunctions can be localized at the boundary, whereas there exist no corresponding normalizable left-eigenfunctions, such that the Green function cannot be expressed in terms of eigenfunctions.

Example: Dirac fermions with non-Hermitian terms.— We consider a continuum model that corresponds to the long distance limit of the non-Hermitian SSH model [32, 41, 65, 66]. It concerns wave functions with two components $\psi(x) = [\psi_1(x), \psi_2(x)]^T$ subject to a Hermitian Dirac Hamiltonian $H_0 = m\sigma_x + (-i\partial_x)\sigma_y$, where σ_x, σ_y are Pauli matrices, m is a real mass parameter (band gap). Let us introduce non-Hermiticity by adding constant antihermitian terms:

$$\hat{H} = \hat{H}_0 + i\gamma\sigma_y, \tag{2}$$

where γ is real. There are three more terms that we could add: $i\gamma_x\sigma_x$, $i\gamma_z\sigma_z$, and $-i\Gamma\mathbb{1}$, where $\mathbb{1}$ is the identity matrix. The first can be absorbed by analytic continuation of the mass m. The second and third vanish if we also impose a chiral symmetry, $\{\hat{H}, \sigma_z\} = 0$, necessary for discussing zero energy boundary eigenstates in one dimension. Thus, the symmetry class is AIII [1] for complex m. For real mass m, $\hat{H}$ is additionally invariant under complex conjugation, placing it in symmetry class BDI, which also implies that eigenvalues occur in complex conjugate pairs.

In the continuum model (2), we have $q_\pm(k) = m \pm (\gamma - ik)$, and the paths described by $q_\pm(k)$ in the complex plane are no longer closed. Still, one can assign a half-integer winding number $\nu_\pm$ [33] that changes whenever a path crosses the origin. Such crossings happen at $\gamma = \pm m$ and we find the topological phase diagram in Fig. 1(a).

Open boundary conditions.— We now consider a system of length L with open boundary conditions

$$\psi_2(0) = 0, \ \psi_1(L) = 0 \tag{3}$$

corresponding to a particular boundary termination of the lattice model. For open boundary conditions, the non-Hermitian terms in both the Dirac-Hamiltonian Eq. (2) and the non-Hermitian SSH model defined below Eq. (1) can be eliminated by a similarity transformation: if $\psi_0(x)$ is an eigenfunction of the Hamiltonian $\hat{H}_0$, then $\psi(x) = e^{\gamma x}\psi_0(x)$ is an eigenfunction of the Hamiltonian $\hat{H}$. From this we see that *all* eigenfunctions are exponentially localized, when $\gamma \neq 0$. This is the non-Hermitian skin effect [39, 41, 55–64].

Bulk and boundary Green function.— To clearly distinguish bulk and boundary, we now focus on Green functions, which are matrix-valued solutions to the equation

$$(E - \hat{H})G(E; x, y) = \mathbb{1}\delta(x - y) \quad . \tag{4}$$

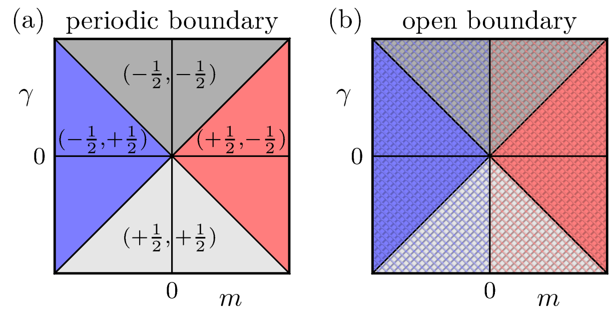

Figure 1. Topological phase diagram of one-dimensional non-Hermitian Dirac fermions with particle-hole symmetry and chiral symmetry. (a) Periodic boundary conditions. A pair of half-integer winding numbers (ν_+, ν_-) distinguishes four phases: Two Hermitian (red and blue) and two genuinely non-Hermitian phases (grey), separated by lines $\gamma = \pm m$. (b) Open boundary conditions. The line $m = 0$ separates phases with a different number of zero energy boundary eigenstates. For the boundary conditions (3), a positive mass implies the existence of a boundary state at each end (red), which are absent for a negative mass (blue). The lines $\gamma = \pm m$ now indicate that the bulk (and boundary) Green function change from exponential decay to exponential growth.

The *bulk Green function* G_{bulk} is defined as the response of an infinite system [54], whereas the Green function G_{open} for open boundary conditions is defined as the solution that satisfies the conditions (3). When we probe the system far away from the boundary, $0 \ll x, y \ll L$, then only the bulk of the system responds, and we expect that both Green functions give the same result. However, when the source is close to the boundary, $y \approx 0$ or $y \approx L$, we expect that reflection at the boundary is important, which is captured in the *boundary Green function*

$$G_{\text{bound}}(E; x, y) := G_{\text{open}}(E; x, y) - G_{\text{bulk}}(E; x - y). \tag{5}$$

It solves the homogeneous equation $(E - \hat{H})G_{\text{bound}}(E; x, y) = 0$. We have used that for a translationally invariant Hamiltonian, the bulk response only depends on the difference $x - y$. If G_0 denotes a Green function of $\hat{H}_0$ for open boundaries, then the corresponding retarded Green function for $\hat{H}$ reads

$$G(E; x, y) = G_0(E + i\eta; x, y)e^{\gamma(x-y)}, \tag{6}$$

with $\eta = 0^+$. We now focus on zero energy, $E = 0$. Then, we find

$$G_{0,\text{bulk}}(i\eta; x, y) = [\theta(-\tilde{x})G_L + \theta(\tilde{x})G_R]e^{-\sqrt{m^2+\eta^2}|\tilde{x}|}, \tag{7}$$

where $\tilde{x} = x - y$, and G_L and G_R are matrices

$$G_s = \mathcal{N}\begin{pmatrix} i\eta & m + \nu_s\sqrt{m^2+\eta^2} \\ m - \nu_s\sqrt{m^2+\eta^2} & i\eta \end{pmatrix} \tag{8}$$

with $s = L, R$, $\nu_{R/L} = \pm 1$, and $\mathcal{N} = 1/(2\sqrt{m^2+\eta^2})$. Thus, we obtain one of our main results: In the phases where the non-Hermitian winding number is nonzero, $|\gamma| > |m|$, the bulk Green function G_{bulk} grows exponentially as $x \to \pm\infty$ while keeping y fixed. For $G_{0,\text{bound}}$ near the left boundary, we find

$$G_{0,\text{bound}}(i\eta, x, y) = G_B e^{-\sqrt{m^2+\eta^2}(x+y)}, \text{ for } x, y \ll L. \tag{9}$$

Here, G_B is the matrix

$$G_B = -G_R \cdot \begin{pmatrix} \frac{m+\sqrt{m^2+\eta^2}}{m-\sqrt{m^2+\eta^2}} & 0 \\ 0 & 1 \end{pmatrix}. \tag{10}$$

Taken together, this yields the decomposition (5).

Boundary eigenstates.— The Green function can be expressed as a sum over eigenstates

$$G(E; x, y) = \sum_n (E - E_n)^{-1} \langle x|\psi_R^n\rangle\langle\psi_L^n|y\rangle. \tag{11}$$

Here, $|\psi_R^n\rangle$ are the so-called right- and $|\psi_L^n\rangle$ the left-eigenstates of the non-Hermitian Hamiltonian, i.e. $H|\psi_R^n\rangle = E_n|\psi_R^n\rangle$ and $H^\dagger|\psi_L^n\rangle = E_n^*|\psi_L^n\rangle$, with $\langle\psi_L^n|\psi_R^m\rangle = \delta_{nm}$ [67]. The contribution $\langle x|\psi_R^n\rangle\langle\psi_L^n|y\rangle$ of an individual eigenstate to the Green function can be extracted as the residue of the pole at $E = E_n$ [68, 69]. For identical positions $x = y$, this residue yields the biorthogonal polarization discussed in Ref. [40]. We now define a *boundary eigenstate* to be the residue of a pole of the *boundary* Green function, and focus on states at zero energy, $E = 0$. For open boundary conditions, our model has only real eigenvalues due to the relation Eq. (6), and we can obtain the residue from the imaginary part of the Green function since $\operatorname{Im} G(E + i0^+; x, y) = -\sum_n \langle x|\psi_R\rangle\langle\psi_L|y\rangle\delta(E - E_n)$ for real E. We find that

$$-\operatorname{Im} {G^{11}}_{\text{bound}}(0, x, y) = A e^{(\gamma-m)x} e^{(-\gamma-m)y}, \quad \text{where } A = \theta(m) 2m/\eta \text{ with } \eta = 0^+. \tag{12}$$

Thus, for $m > 0$, the boundary Green function has an isolated pole at zero energy, whose associated eigenstate is $\langle x|\psi_R^0\rangle = e^{(\gamma-m)x}$ and $\langle\psi_L^0|y\rangle = e^{(-\gamma-m)y}$. The spatial shape changes dramatically from exponentially localized to exponentially growing and vice versa whenever $\gamma = \pm m$. In contrast, for $m < 0$, no boundary eigenstate is found. Thus, the number of zero energy boundary eigenstates does not change during the topological phase transition at $\gamma = \pm|m|$ for periodic boundary conditions [Fig. 1(b)], and the bulk-boundary correspondence breaks down.

Bulk-periodic correspondence.— The traditional view on the bulk-boundary correspondence actually comprises two separate logical steps: it relates i) the bulk to the boundary Green function, and ii) the Green function G_{period} for periodic boundary conditions to that for the bulk of an infinite system: In the limit of large system size, both agree if the bulk Green function decays spatially [Fig. 2(a)]; this allows us to use topological invariants of the Bloch Hamiltonian (1) to characterize an infinite bulk. In non-Hermitian systems, step i) is unproblematic, but step ii) may fail. To better distinguish them, we propose to narrow the name *bulk-boundary correspondence* to refer only to the first step, and to call the second step the *bulk-periodic correspondence*.

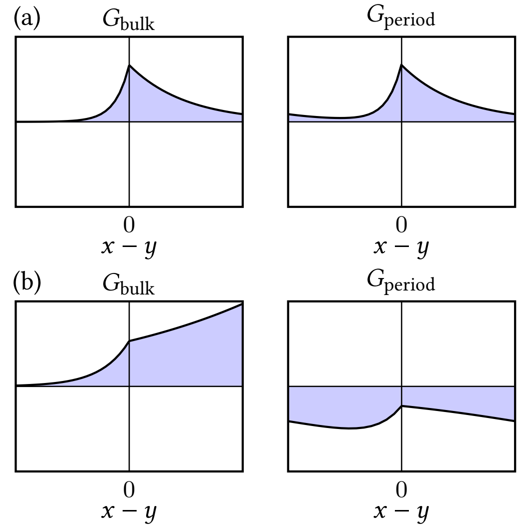

Figure 2. Breakdown of the bulk-periodic correspondence. (a) If the bulk Green function decays spatially, then both bulk and periodic Green function agree. (b) If the bulk Green function grows spatially, then the periodic Green function has to change drastically in order to accommodate periodic boundary conditions.

Indeed, for our model in the regime $|\gamma| > |m|$, the bulk-periodic correspondence breaks down, because the periodic Green function decays, while the bulk Green function grows exponentially. [Fig. 2(b)] This growth also explains the exponential sensitivity to small perturbations seen in Ref. [44]. For periodic boundary conditions $\psi(-L/2) = \psi(+L/2)$, and using the results Eqs. (6) and (7) for the bulk Green function, we find

$$G_{\text{period}}(0; x, 0) = G_{\text{bulk}}(0; x, 0) + G_L \frac{e^{\kappa_L x}}{e^{\kappa_L L} - 1} + G_R \frac{e^{\kappa_R x}}{e^{-\kappa_R L} - 1}. \tag{13}$$

with $\kappa_{L/R} = \gamma \pm \sqrt{m^2 + \eta^2}$. In the limit of large system size, $L \gg |x|$, the two additional terms vanish if only if the exponents satisfy $\kappa_L > 0$ and $\kappa_R < 0$, i.e. if the bulk Green function decays spatially [Fig. 2].

If we focus on bulk growth and disregard boundary eigenstates, we no longer require symmetry class AIII. Then, we find our main result, which holds both with and without symmetry (class A): If the non-Hermitian winding number is nonzero, then the bulk Green function at zero energy grows spatially. For example, consider