Classification of massive Dirac models with generic non-Hermitian perturbations

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We present a systematic investigation of d-dimensional massive Dirac models perturbed by three different types of non-Hermitian terms: (i) non-Hermitian terms that anti-commute with the Dirac Hamiltonian, (ii) non-Hermitian kinetic terms, and (iii) non-Hermitian mass terms. We show that these perturbations render the Hamiltonian either intrinsically or superficially non-Hermitian, depending on whether the non-Hermiticity can be removed by non-unitary similarity transformations. A two-fold duality is revealed for the first two types of non-Hermitian perturbations: With open boundary conditions non-Hermitian terms of type (i) give rise to intrinsic non-Hermiticity, while terms of type (ii) lead to superficial non-Hermiticity. Vice versa, with periodic boundary conditions type-(i) perturbations induce superficial non-Hermiticity, while type-(ii) perturbations generate intrinsic non-Hermiticity. Importantly, for the type-(i) and type-(ii) terms the intrinsic non-Hermiticity manifests itself by exceptional spheres of dimension (d – 2) in the surface and bulk band structures, respectively. Type-(iii) perturbations, in contrast, render the Hamiltonian always intrinsically non-Hermitian, independent of the boundary condition, but do not induce exceptional spheres in the band structure. For each of the three perturbations we study the band topology, discuss the topological surface states, and briefly mention the relevance for potential applications.

The fields of non-Hermitian physics and topological materials have recently intertwined to create the new research direction of non-Hermitian topological phases. As a result of the joint efforts from both fields, fascinating new discoveries have been made, both at the fundamental level and with respect to applications [1–22]. For instance, topological exceptional points have been found in one-dimensional non-Hermitian lattices [12–15] and in non-Hermitian Chern insulators [16–19]. Exceptional rings and bulk Fermi arcs have been discovered in non-Hermitian topological semimetals [20–22]. At these exceptional points and rings, two or more eigenstates become identical and self-orthogonal, leading to a defective Hamiltonian with nontrivial Jordan normal form [23]. These exceptional manifolds have many interesting applications, e.g., enhanced sensitivity of microwavcavity sensors [1], single-mode lasing of photonic devices [2, 5], and stopping of light in coupled optical waveguides [6]. Furthermore, it has been shown that non-Hermitian topological Hamiltonians provide useful descriptions of strongly correlated materials in the presence of disorder or dissipation [23–33]. This has given new insights into the Majorana physics of semiconductor-superconductor nanowires [34] and into the quantum oscillations of SmB6 [35–36].

Despite these recent activities, a general framework for the study and the complete classification of non-Hermitian topological phases is still absent. In particular, the formulation of bulk topological invariants, the associated bulk-boundary correspondence, and the role of boundary conditions are still unclear for non-Hermitian topological phases, although various attempts have been made with partial successes for certain special cases [12–19, 33, 37–38]. Since most non-Hermitian experimental systems can be faithfully captured by Dirac Hamiltonians with small non-Hermitian perturbations [2, 7, 39–44], a systematic investigation of non-Hermitian Dirac models would be particularly valuable. This would be not only of fundamental interest, but could also inform the design of new applications.

In this Letter, we present a systematic investigation of d-dimensional massive Dirac Hamiltonians perturbed by small non-Hermitian terms. We show that these can be either intrinsically or superficially non-Hermitian, depending on whether the non-Hermiticity can be removed by a similarity transformation with open or periodic boundary conditions. According to the Clifford algebra, general non-Hermitian terms can be categorized into three different types: (i) non-Hermitian terms that anti-commute with the whole Dirac Hamiltonian, (ii) kinetic non-Hermitian terms, and (iii) non-Hermitian mass terms. Remarkably, we find a two-fold duality for the first two types of non-Hermitian perturbations: Dirac models perturbed by type-(i) terms are superficially non-Hermitian with periodic boundary conditions (PBCs), but intrinsically non-Hermitian with open boundary conditions (OBCs). Vice versa, Dirac models with type-(ii) terms are intrinsically non-Hermitian with PBCs, but superficially non-Hermitian with OBCs. Interestingly, for type-(i) and type-(ii) terms the non-Hermiticity leads to (d – 2)-dimensional exceptional spheres in the surface and bulk band structures, respectively. Type-(iii) terms, on the other hand, induce intrinsic non-Hermiticity both for OBCs and PBCs, but with a purely real surface-state spectrum and no exceptional spheres.

General formalism.— We begin by discussing some general properties of non-Hermitian physics. First, we recall that in Hermitian physics only unitary transfor-
mations of the Hamiltonian are considered, because only these preserve the reality of the expectation values. In non-Hermitian physics, however, the Hamiltonian can be similarity transformed, $H \rightarrow V^{-1}HV$, by any invertible matrix $V$, which is not necessarily unitary but is required to be local. For this reason, a large class of non-Hermitian Hamiltonians $H$ can be converted into Hermitian ones by non-unitary similarity transformations, i.e.,

$$V^{-1}HV = H', \quad H'^\dagger = H'.\quad (1)$$

Using this observation, we call Hamiltonians whose non-Hermiticity can or cannot be removed by the above transformation as superficially or intrinsically non-Hermitian, respectively.

For non-interacting local lattice models, which is our main focus here, $H$ is a quadratic form, whose entries are specified as $H_{(r\alpha),(r'\alpha')}$ with $r$ the positions of the unit cells and $\alpha$ a label for internal degrees of freedom. Correspondingly, the similarity transformation has matrix elements $V_{(r\alpha),(r'\alpha')}$. By the locality condition, the matrix elements $H_{(r\alpha),(r'\alpha')}$ and $V_{(r\alpha),(r'\alpha')}$ are required to tend to zero sufficiently fast as $|r - r'| \rightarrow \infty$. If $H$ can be converted into a Hermitian Hamiltonian by a local transformation $V$, its eigenvalues are necessarily real. Conversely, any local lattice Hamiltonian with real spectrum is either entirely Hermitian or superficially non-Hermitian [45].

A characteristic feature of non-Hermitian lattice models is the existence of exceptional points in parameter space, where one or multiple eigenvalues become identical, leading to a non-diagonalizable Hamiltonian. However, it is important to note that such exceptional points are not dense in parameter space. I.e., there exist arbitrarily small perturbations which remove the exceptional points, rendering the Hamiltonian diagonalizable. One such perturbation relevant for lattice models are the boundary conditions [15-46], which modify the hopping amplitudes between opposite boundaries. For a general classification of non-Hermitian Hamiltonians, it is therefore essential to distinguish between different types of boundary conditions, in particular OBCs and PBCs. With PBCs and assuming translation symmetry, we can perform a Fourier transformation of Eq. (1) to obtain

$$H'(k) = V^{-1}kH(k)V(k).$$

Here, $V(k)$ is assumed to be local in momentum space. It is worth noting that the locality in momentum space is essentially different from that in real space. Generically, the Fourier transform of $V(k)$, $V_{r,r'} = \sum_k V(k)e^{ik(r-r')}$, is not local in general.

**Non-Hermitian Dirac Hamiltonians.**— We now apply the above concepts to non-Hermitian Dirac models of the form $H = H_0 + \lambda U$, where $H_0$ is a Hermitian Dirac Hamiltonian with mass $M$, and $U$ a non-Hermitian perturbation with $\lambda \ll M$. Assuming PBCs in all directions, we consider the following Hermitian Dirac Hamiltonian on the $d$-dimensional cubic lattice

$$H_0(k) = \sum_{i=1}^d \sin k_i \Gamma_i + (M - \sum_{i=1}^d \cos k_i) \Gamma_{d+1}, \quad (2)$$

where $\Gamma_\mu$ denote the gamma matrices that satisfy $\{\Gamma_\mu, \Gamma_\nu\} = 2\delta_{\mu\nu}$ and $M$ is the real mass parameter. With OBCs in the $j$th direction and PBCs in all other directions, the Hamiltonian reads

$$H_0(\mathbf{\bar{k}}) = \frac{1}{2i} (\mathbf{\bar{S}} - \mathbf{\bar{S}}^\dagger) \otimes \Gamma_j - \frac{1}{2} (\mathbf{\bar{S}} + \mathbf{\bar{S}}^\dagger) \otimes \Gamma_{d+1} + \mathbb{I}_{N_j} \otimes (\sum_{i \neq j} \sin k_i \Gamma_i + (M - \sum_{i \neq j} \cos k_i) \Gamma_{d+1}), \quad (3)$$

where $\mathbf{\bar{k}}$ denotes the vector of all momenta except $k_j$, $\mathbf{\bar{S}}_{ij} = \delta_{i,j+1}$ is the right-translational operator, and $N_j$ stands for the number of layers in the $j$th direction. From the above two equations it is now clear that, according to the Clifford algebra, there exist only the three types of non-Hermitian perturbations discussed in the introductions. We will now study these individually.

**Non-Hermitian terms of type (i).**— We start with non-Hermitian terms that anti-commute with the Dirac Hamiltonian $H_0$. Such non-Hermitian terms are possible for all Altland-Zirnbauer classes with chiral symmetry [47-48], in which case they are given by the chiral

![FIG. 1](image-url)
operator $\Gamma$. With PBCs the Hamiltonian perturbed by these type-(i) terms is expressed as

$$H(k) = H_0(k) + i\lambda\Gamma,$$  

where $\Gamma$ is an additional gamma matrix with $\{\Gamma, H_0(k)\} = 0$ and $\lambda$ a real parameter. The spectrum of $H(k)$ is given by $E(k) = \pm \sqrt{d^2(k) - \lambda^2}$ with $d^2(k) = H_0^2(k)$, which is completely real for all $k$, provided that $|\lambda|$ is smaller than the energy gap of $H_0$. Thus, Hamiltonian \[4\] with $\lambda \ll M$ is only superficially non-Hermitian and we can remove the non-Hermitian term by a similarity transformation. The corresponding transformation matrix $V(k)$ can be derived systematically by noticing that the flattened Hamiltonian $H_0(k) = H_0(k)/d(k)$ and $\Gamma$ form a Clifford algebra and, thus, $i[H_0(k), \Gamma]/4$ generates rotations of the plane spanned by $H_0(k)$ and $\Gamma$. Hence, the explicit expression of the transformation matrix is $V(k) = \exp[-\frac{i}{2}H_0(k)\Gamma\eta(k)]$, with $e^{i\eta(k)} = \sqrt{(d(k) + \lambda)/d(k) - \lambda}$. From Eq. \[1\] it follows that the transformed Hamiltonian is $H'(k) = \sqrt{1 - \lambda^2/d^2(k)}H_0(k)$, which is manifestly Hermitian for $\lambda \ll M$.

With OBCs, on the other hand, type-(i) perturbations lead to intrinsic non-Hermiticity, provided the Dirac Hamiltonian $H_0$ is in the topological phase. This is because the topological boundary modes acquire complex spectra due to the non-Hermitian term $i\lambda\Gamma$, even for infinitesimally small $\lambda$. To see this, we first observe that for any eigenstate $\psi_0$ of $H_0$ with energy $E_0$, $\Gamma\psi_0$ is also an eigenstate of $H_0$, but with opposite energy $-E_0$. Applying chiral perturbation theory to $H = H_0 + i\lambda\Gamma$, we find that since $i\lambda\Gamma$ scatters $\psi_0$ into $\Gamma\psi_0$, eigenstates of $H$ can be expressed as superpositions of $\psi_0$ and $\Gamma\psi_0$. Explicitly, we find that the eigenstates of $H$ are $\psi_j = \psi_0 + c_{\pm}i\lambda\psi_0$, with $c_{\pm} = iE_0/\lambda \pm \sqrt{1 - E_0^2/\lambda^2}$ and energy $E_{\pm} = \pm \sqrt{E_0^2 - \lambda^2}$. This analysis holds in particular also for the topological boundary modes of $H_0$, which are massless Dirac fermions with linear dispersions. Consequently, even for arbitrarily small $\lambda$, there exists a segment in the spectrum of $H$ around $E = 0$ with purely imaginary eigenenergies.

To make this more explicit, we can derive a low-energy effective theory for the boundary modes, by projecting the bulk Hamiltonian onto the boundary space. Generally, the boundary theory is of the form $H_b(k) = \sum_{i\neq j} k_i\gamma_i^* + i\lambda\gamma_j^*$, with the first term describes the boundary massless Dirac fermions of $H_0$. The matrices $\gamma_i^*$ and $\gamma_j$ are the projections of $\Gamma_i$ and $\Gamma_j$, respectively, onto the boundary space, and satisfy $\{\gamma_i^*, \gamma_j\} = 0$. With this, we find that the boundary spectrum is $E_b = \pm \sqrt{|k|^2 - \lambda^2}$, and that there exists a $(d - 2)$-dimensional exceptional sphere of radius $|k| = \lambda$ in the boundary Brillouin zone, which separates eigenstates with purely real and purely complex energies from each other.

As an aside, we remark that even arbitrarily large non-Hermitian terms $i\lambda\Gamma$ cannot remove the topological surface state. The reason for this is that $i\lambda\Gamma$ is a chiral operator, which acts only within a unit cell and does not couple different sites. In other words, the expectation value of the position operator $X_i$ is independent of $\lambda$, i.e., \[\frac{d}{dk}(\langle \psi_{k_i}^\dagger \phi \psi_{k_i}\rangle) = 0\] with $\langle \psi_{k_i}^\dagger \phi \psi_{k_i}\rangle$ the left and right eigenstates of $H$, respectively.

Let us now illustrate the above general considerations by considering an example, $H_{\text{TI}}(k) = k_x\Gamma_1 + \sin k_y\Gamma_2 + (M - \cos k_x - \cos k_y)\Gamma_3 + i\lambda\Gamma_4$, with $\Gamma_j$ the $4 \times 4$ Dirac gamma matrices, which describes a topological superconductor in class DIII or a topological insulator in class AII \[43\]. The energy spectra of $H_{\text{TI}}$ with periodic and open boundary conditions are shown in Figs. \[\text{a}\] and \[\text{b}\], respectively, see Supplemental Material (SM) \[49\] for details. We observe that the bulk spectrum is purely real, while the surface spectrum is complex with two exceptional points of second order located at $k_x = \pm \arcsin|\lambda|$.

**Non-Hermitian terms of type (ii).**—We proceed by considering non-Hermitian kinetic terms added to $H_0$ with PBCs. The effects of these non-Hermitian terms can be most clearly seen by studying the continuous version of Eq. \[2\], namely

$$H(k) = H_0(k) + i\lambda\Gamma_j = \sum_{i=1}^d k_i\Gamma_i + m\Gamma_{d+1} + i\lambda\Gamma_j,$$  

with $1 \leq j \leq d$ and $\lambda$ real. The energy spectrum of $H(k)$, $E(k) = \pm \sqrt{\sum_{i \neq j} k_i^2 + (k_j + i\lambda)^2 + m^2}$, is complex and exhibits exceptional points on the $(d - 2)$-dimensional sphere $\sum_{i \neq j} k_i^2 + m^2 = \lambda^2$ within the $k_j = 0$ plane. Hence, $H(k)$ with PBCs is intrinsically non-Hermitian.

To study the case of OBCs we consider $H(k)$ in a slab geometry with surface perpendicular to the $j$th direction. The energy spectrum in this geometry is obtained from $H(\hat{k}, -i\partial_j)$, i.e., by replacing $k_j$ by $-i\partial_j$ in Eq. \[5\]. Then, it is obvious that the non-Hermitian term $i\lambda\Gamma_j$ can be removed by the similarity transformation $V = e^{i\lambda\partial_j}$. That is, $e^{-i\lambda\partial_j}H(\hat{k}, -i\partial_j)e^{i\lambda\partial_j} = H_0(\hat{k}, -i\partial_j)$, which is manifestly Hermitian. Accordingly, $H(\hat{k}, -i\partial_j)$ has real spectrum and its eigenstates are related to those of $H_0(\hat{k}, -i\partial_j)$ by $\psi(x_j, k) = e^{i\lambda x_j}\psi_0(x_j, k)$. We conclude that continuous Dirac models perturbed by non-Hermitian kinetic terms are superficially non-Hermitian with OBCs, but intrinsically non-Hermitian with PBCs. The same holds true for lattice Dirac models.

To exemplify this, we consider the lattice Dirac model of Eq. \[3\] perturbed by the non-Hermitian term $i\lambda\Gamma_j$, i.e., $H(k) = H_0(k) + \mathbb{I} \otimes i\lambda\Gamma_j$. This Hamiltonian can be...
Here, the modes of Eq. (3) are perturbed by the non-Hermitian mass term \( \lambda \sum \delta^j \), with periodic and open boundary conditions, respectively. The parameters are chosen as \( M = 1.5 \) and \( \lambda = 0.3 \). Solid and dotted lines represent bulk and surface states, respectively.

Transformed to (see SM [49] for details)

\[
H'(\vec{k}) = \frac{1}{2i} (\vec{S} - \vec{S}^\dagger) \otimes \Gamma_j - \frac{1}{2} (\vec{S} + \vec{S}^\dagger) \otimes \Gamma_{d+1} + \mathbb{I} \otimes (\sum_{i \neq j} \sin k_i \Gamma_i + \sqrt{M_k^2 - \lambda^2 \Gamma_{d+1}}), \tag{6}
\]

by the similarity transformation \( V = \text{diag} \{1, \alpha, \cdots, \alpha^{N_i-1} \} \otimes [(1 + \alpha) \mathbb{I} + i(1 - \alpha) \Gamma_j, \Gamma_{d+1}] \). Here, \( \alpha = \sqrt{(M_k - \lambda)/(M_k + \lambda)} \) and \( M_k = M - \sum_{i \neq j} \cos k_i \). Eq. (6) is manifestly Hermitian for \( \lambda \ll M \). As a concrete example, we set in Eq. (6) \( d = 2 \) with \( \Gamma_j \) the Dirac gamma matrices, which describes a two-dimensional topological insulator. The energy spectra for this case with periodic and open boundary conditions are shown in Figs. 3(c) and (d), respectively.

Non-Hermitian terms of type (iii). — Finally, we examine the effects of non-Hermitian mass terms. For that purpose, we add \( i\lambda \Gamma_{d+1} \) to Eqs. (2) or (3), which is equivalent to assuming that the mass \( M \) is complex. Hence, the energy spectrum is always complex independent of the boundary conditions, see SM [49]. Thus, massive Dirac models perturbed by non-Hermitian mass terms are intrinsically non-Hermitian, both for open and periodic boundary conditions. Furthermore, we find that there are no exceptional points, not in the bulk and not in the surface band structure. Indeed, remarkably, topological boundary modes are unaffected by type-(iii) perturbations and keep their purely real energy spectra.

To demonstrate this explicitly, we solve for the boundary modes of Eq. (3) perturbed by \( i\lambda \Gamma_{d+1} \). I.e., we solve \( (H_0(\vec{k}) + i\lambda \Gamma_{d+1}) |\psi_{\vec{k}}\rangle = E |\psi_{\vec{k}}\rangle \) with \( |\psi_{\vec{k}}\rangle \) the ansatz for the left eigenvector of the boundary mode, \( |\psi_{\vec{k}}\rangle = \sum_{i=1}^{N_i} \beta^i |\xi_{\vec{k}}\rangle \), where \( |\xi_{\vec{k}}\rangle \) is a spinor, \( i \) labels the lattice sites along the \( j \)th direction, and \( \beta \) is a scalar with \( |\beta| < 1 \) (see SM [49] for details). By solving this Schrödinger equation we find that \( \beta = M - \sum_i \cos k_i + i\lambda \) and that the boundary mode is an eigenstate of \( i\Gamma_{d+1} \Gamma_j \) with eigenvalue \( +1 \). Hence, the projector \( P \) onto the boundary space is given by \( P = (1 + i\Gamma_{d+1} \Gamma_j)/2 \) and the effective boundary Hamiltonian is obtained by \( H_0(\vec{k}) = P(H_0(\vec{k}) + i\lambda \Gamma_{d+1})P \), with \( \vec{k} \) satisfying \( |\beta| = |M - \sum_i \cos k_i + i\lambda| < 1 \). Since \( \Gamma_{d+1} \) anti-commutes with \( P \), the non-Hermitian perturbation \( i\lambda \Gamma_{d+1} \) vanishes under the projection. Thus, the effective boundary Hamiltonian becomes \( H_0(\vec{k}) = \sum_{i \neq j} \sin k_i \gamma^i \), with \( \gamma^i = P \Gamma_j P \), whose spectrum is manifestly real. We note that while the effective boundary Hamiltonian is not altered by the non-Hermitian mass term \( i\lambda \Gamma_{d+1} \), the range of \( \vec{k} \) in which the boundary modes exist is changed to \( |M - \sum_i \cos k_i + i\lambda| < 1 \).

Conclusions and Discussions. — In summary, we systematically investigated non-Hermitian massive Dirac models with three different types of non-Hermitian terms. We find that there is a two-fold duality for the first two types of terms, which lead either to superficial or intrinsic non-Hermiticity, depending on the boundary conditions. Moreover, the first and second type of terms give rise to exceptional points in the surface and bulk band structures, respectively. Terms of the third type, however, always induce intrinsic non-Hermiticity, but do not produce exceptional points. Our findings can be used as guiding principles for the design of applications in, e.g., photonic devices. For example, our analysis shows that single mode lasing [2–5], which utilizes bulk exceptional points, is only possible in Dirac models perturbed by the second type of non-Hermitian terms. Sensors, on the other hand, which make use of surface exceptional points, can be designed using Dirac models with the first type of non-Hermitian terms. We emphasize, that the exceptional points are extremely sensitivity to the boundary conditions, as they are bare (i.e., not dense) in parameter space. That is, infinitesimally small perturbations can change them into regular points, a fact that can be exploited for sensor applications. This important fact deserves further investigations, both from a fundamental and applications point of view.
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[49] See Supplemental Material for the solution of the two-dimensional topological insulator with the three different types of non-Hermitian terms, the derivation of the similarity transformation of the massive Dirac model with OBCs perturbed by non-Hermitian kinetic terms, and the calculation of the boundary modes of the Dirac model with non-Hermitian mass term.
Supplemental Material

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In this Supplemental Material, we solve the lattice model of two dimensional topological insulator with non-Hermitian anti-commuting term in both momentum and real space with open boundary conditions (Sec. I), derive the similarity transformation for the general Dirac model with non-Hermitian kinetic terms in real space (Sec. II), and calculate the boundary states of the generic Dirac model with non-Hermitian mass terms (Sec. III).

I. 2D TOPOLOGICAL INSULATOR WITH NON-HERMITIAN ANTI-COMMUTING TERM

We start with the Hermitian lattice model of 2D topological insulator,

$$\mathcal{H}_{\text{TI,0}}(k) = \sin k_x \Gamma_1 + \sin k_y \Gamma_2 + (M - \cos k_x - \cos k_y) \Gamma_3,$$

where the five gamma matrices are $\Gamma_i = \sigma_i \otimes \tau_1$, $\Gamma_4 = \sigma_0 \otimes \tau_1$, $\Gamma_5 = \sigma_0 \otimes \tau_2$ ($i = 1, 2, 3$), with $\sigma_i$ and $\tau_i$ Pauli matrices. The energy spectrum is $E_{\text{TI,0}}(k) = \pm d_{\text{TI}}(k)$, with $d_{\text{TI}}^2(k) = \sin^2 k_x + \sin^2 k_y + (M - \cos k_x - \cos k_y)^2$. The eigenstates are found to be,

$$\begin{align*}
|\pm, \uparrow\rangle &= \frac{1}{\sqrt{2d_{\text{TI}}}} \left( \sin k_x - i \sin k_y, -M(k), 0, d_{\text{TI}} \right)^T, \\
|\pm, \downarrow\rangle &= \frac{1}{\sqrt{2d_{\text{TI}}}} \left( M(k), \sin k_x + i \sin k_y, d_{\text{TI}}, 0 \right)^T, \\
|\mp, \uparrow\rangle &= \frac{1}{\sqrt{2d_{\text{TI}}}} \left( -\sin k_x + i \sin k_y, M(k), 0, d_{\text{TI}} \right)^T, \\
|\mp, \downarrow\rangle &= \frac{1}{\sqrt{2d_{\text{TI}}}} \left( -M(k), -\sin k_x + i \sin k_y, d_{\text{TI}}, 0 \right)^T,
\end{align*}$$

with $M(k) = M - \cos k_x - \cos k_y$ and $T$ the matrix transposition. The system is topologically non-trivial for $M \in (-2, 2)$.

Including the non-Hermitian anti-commuting perturbation $i\lambda \Gamma_4$, the Hamiltonian becomes

$$\mathcal{H}_{\text{TI}}(k) = \mathcal{H}_{\text{TI,0}}(k) + i\lambda \Gamma_4.$$  \hfill (S3)

According to our theory, the non-Hermitian perturbation scatters eigenstates $\psi_0$ to $\Gamma_4 \psi_0$. The spectrum becomes $E_{\text{TI}}(k) = \pm \sqrt{d_{\text{TI}}^2(k) - \lambda^2}$, and the corresponding eigenstates are modified as $\psi_{\pm} = \psi_0 + (iE_{\text{TI},0}/\lambda \pm \sqrt{1 - E_{\text{TI},0}^2/\lambda^2})\Gamma_4 \psi_0$, with $\psi_0$ given in Eq. (S2).

For $d_{\text{TI}}^2(k) > \lambda^2$, the spectrum is purely real in momentum space, thus according to the similarity transformation constructed below Eq. (4) in the main text, the Hamiltonian in Eq. (S3) can be converted to be Hermitian by

$$\mathcal{V}(k)^{-1} \mathcal{H}_{\text{TI}}(k) \mathcal{V}(k) = \sqrt{1 - \frac{\lambda^2}{d_{\text{TI}}^2(k)}} \mathcal{H}_{\text{TI,0}}(k),$$

where $\mathcal{V}(k) = \exp[-\frac{i}{2} \mathcal{H}_{\text{TI,0}}(k) \Gamma_4 \eta_{\text{TI}}(1)/d_{\text{TI}}(k)]$, with $e^{\eta_{\text{TI}}(k)} = \sqrt{(d_{\text{TI}}(k) + \lambda)/(d_{\text{TI}}(k) - \lambda)}$. The matrix form of $\mathcal{V}(k)$ is,

$$\mathcal{V}(k) = \cosh \frac{\eta_{\text{TI}}(k)}{2} - i \sinh \frac{\eta_{\text{TI}}(k)}{2} \mathcal{H}_{\text{TI,0}}(k) \Gamma_4 / d_{\text{TI}}(k).$$

Taking open boundary conditions in $y$ direction with $N_y$ layers, the real space Hamiltonian reads

$$H_{\text{TI}}(k_x) = \frac{1}{2i} \left( \hat{S} - \hat{S}^\dagger \right) \otimes \Gamma_2 - \frac{1}{2} \left( \hat{S} + \hat{S}^\dagger \right) \otimes \Gamma_3 + \sum_{N_y} \otimes \left( \sin k_x \Gamma_1 + (M - \cos k_x) \Gamma_3 \right) + \sum_{N_y} \otimes i\lambda \Gamma_4.$$  \hfill (S6)

Here $\hat{S}$ and $\hat{S}^\dagger$ are the forward and backward translation operators in $y$ direction, which let $\hat{S}|i\rangle = |i + 1\rangle$ and $\hat{S}^\dagger|i\rangle = |i - 1\rangle$, where $i$ labels the $i$th site in the $y$ direction. As $\langle i|\hat{S}|j\rangle = \delta_{i,j+1}$, the corresponding matrices...
are,

\[
\hat{S} = \begin{pmatrix}
0 & 0 & 0 & \cdots & 0 \\
1 & 0 & 0 & \cdots & 0 \\
0 & 1 & 0 & \cdots & 0 \\
0 & 0 & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 1
\end{pmatrix}, \quad \hat{S}^\dagger = \begin{pmatrix}
0 & 1 & 0 & \cdots & 0 \\
0 & 0 & 1 & \cdots & 0 \\
0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 0
\end{pmatrix},
\]

(S7)

with dimension \(N_y\).

Though the translational symmetry is violated in \(y\) direction, it is still preserved in \(x\) direction. We use the ansatz \(|\psi_{k_n}\rangle = \sum_{i=1}^{N_y} \beta^i |i\rangle \otimes |\xi_{k_n}\rangle\) with \(|\beta| < 1\) for the boundary states. The Shrödinger equation for the real space system leads the relations for the bulk \((1 < i < N_y)\),

\[
\left[ \sin k_x \Gamma_1 + \frac{1}{2i} (\beta - \beta^{-1}) \Gamma_2 + (M - \cos k_x) \right. \\
\left. - \frac{1}{2} (\beta + \beta^{-1}) \Gamma_3 + i \lambda \Gamma_4 \right]|\xi_{k_n}\rangle = \hat{E}_{k_n} |\xi_{k_n}\rangle,
\]

and for the boundary at \(i = 1:\)

\[
\left[ \sin k_x \Gamma_1 + \frac{1}{2i} \beta \Gamma_2 + (M - \cos k_x - \frac{1}{2} \beta) \Gamma_3 \\
+ i \lambda \Gamma_4 \right]|\xi_{k_n}\rangle = \hat{E}_{k_n} |\xi_{k_n}\rangle.
\]

(S8)

Taking the difference between these two relations, we obtain a simpler constraint,

\[
i \Gamma_3 \Gamma_2 |\xi_{k_n}\rangle = |\xi_{k_n}\rangle,
\]

(S10)

which means the boundary states correspond to the positive eigenvalue of \(i \Gamma_3 \Gamma_2\), from which we can construct the projector,

\[
P = \frac{1}{2} (1 + i \Gamma_3 \Gamma_2).
\]

(S11)

Applying this projector to Eq. (S9), we have

\[
(\sin k_x \Gamma_1 + i \lambda \Gamma_4) |\xi_{k_n}\rangle = \hat{E}_{k_n} |\xi_{k_n}\rangle.
\]

(S12)

Under the relation of Eq. (S10), Eq. (S9) becomes

\[
[ \sin k_x \Gamma_1 + (M - \cos k_x - \beta) \Gamma_3 + i \lambda \Gamma_4 ] |\xi_{k_n}\rangle = \hat{E}_{k_n} |\xi_{k_n}\rangle,
\]

and its difference with Eq. (S12) yields

\[
\beta = M - \cos k_x.
\]

(S13)

The boundary effective Hamiltonian can be obtained after the projection,

\[
\mathcal{H}_{T1,b}(k_x) = P \mathcal{H}_{T1}(k) P = \sin k_x \gamma^1 + i \lambda \gamma^4,
\]

(S14)

with \(\gamma^1 = \Gamma_1 P \Gamma_1 P^\dagger\) and \(\gamma^4 = \Gamma_4 P \Gamma_4 P^\dagger\), for \(k_x\) satisfying \(|\beta| = |M - \cos k_x| < 1\). The boundary spectrum is \(\mathcal{E}_{T1,b}(k_x) = \pm \sqrt{\sin^2 k_x - \lambda^2}\). For \(|\lambda| < 1\), exceptional points emerge at \(k_x = \pm \arcsin |\lambda|\).

In the main text, the non-Hermitian potential is relatively small and thus can be treated as perturbation. In FIG. S1, we increase the magnitude of the non-Hermitian potential. With increasing \(\lambda\), the bulk system become gapless with both real and imaginary spectrum (a), and gapless with purely imaginary spectrum (c). Their corresponding boundary states are denoted by dotted lines in (b) and (d), which exist even when the bulk becomes gapless.

II. SIMILARITY TRANSFORMATION FOR THE REAL SPACE DIRAC MODEL WITH NON-HERMITIAN KINETIC TERMS

The lattice Dirac model with non-Hermitian kinetic perturbation reads,

\[
H(\hat{k}) = \frac{1}{2i} (\hat{S} - \hat{S}^\dagger) \otimes \Gamma_j - \frac{1}{2} (\hat{S} + \hat{S}^\dagger) \otimes \Gamma_{d+1} + \Gamma_N \otimes \left( \sum_{i \neq j} \sin k_i \Gamma_i + (M - \sum_{i \neq j} \cos k_i) \Gamma_{d+1} + i \lambda \Gamma_j \right),
\]

(S15)

which is superficially non-Hermitian in real space. Note that for the part \((M - \sum_{i \neq j} \cos k_i) \Gamma_{d+1} + i \lambda \Gamma_j\) in the above Hamiltonian, the non-Hermitian term \(i \lambda \Gamma_j\) can be regarded as a non-Hermitian anti-commuting perturbation. Hence, we can first convert this part to be Hermitian by the following similarity transformation,

\[
\rho_i^{-1} [(M - \sum_{i \neq j} \cos k_i) \Gamma_{d+1} + i \lambda \Gamma_j] \rho_i = \sqrt{M_k^2 - \lambda^2 \Gamma_{d+1}},
\]

(S16)

with \(M_k = M - \sum_{i \neq j} \cos k_i\). Here \(\rho_i = (1 + \alpha) I + i (1 - \alpha) \Gamma_j \Gamma_{d+1}\), with \(\alpha = \sqrt{(M_k - \lambda) / (M_k + \lambda)}\), and its inverse is \(\rho_i^{-1} = \frac{1}{1 + \alpha} [(1 + \alpha) I - i (1 - \alpha) \Gamma_j \Gamma_{d+1}]\). Next we turn to the remaining terms in Eq. (S15) with non-trivial spatial parts,

\[
\frac{1}{2i} (\hat{S} - \hat{S}^\dagger) \otimes \Gamma_j - \frac{1}{2} (\hat{S} + \hat{S}^\dagger) \otimes \Gamma_{d+1} = \hat{S} \otimes \left( \frac{1}{2i} \Gamma_j - \frac{1}{2} \Gamma_{d+1} \right) - \hat{S}^\dagger \otimes \left( \frac{1}{2i} \Gamma_j + \frac{1}{2} \Gamma_{d+1} \right).
\]

(S17)

The operator \(\rho_i\) acts on the internal degree parts of terms in above equation as

\[
\hat{S} \otimes \rho_i^{-1} \left( \frac{1}{2i} \Gamma_j - \frac{1}{2} \Gamma_{d+1} \right) \rho_i = \alpha \hat{S} \otimes \left( \frac{1}{2i} \Gamma_j - \frac{1}{2} \Gamma_{d+1} \right),
\]

(S18)

\[
\hat{S}^\dagger \otimes \rho_i^{-1} \left( \frac{1}{2i} \Gamma_j + \frac{1}{2} \Gamma_{d+1} \right) \rho_i = \frac{1}{\alpha} \hat{S}^\dagger \otimes \left( \frac{1}{2i} \Gamma_j + \frac{1}{2} \Gamma_{d+1} \right).
\]

(S19)

We can construct the spatial part similarity transformation \(\rho_S = \text{diag}(1, \alpha, \alpha^2, \ldots, \alpha^{N_y-1})\), which enables the
transformation
\[\rho_S^{-1}(\alpha S)\rho_S = \hat{S}, \quad (S20)\]
\[\rho_S^{-1}(\frac{1}{\alpha^*} \hat{S}^\dagger)\rho_S = \hat{S}^\dagger. \quad (S21)\]

Finally, the full similarity transformation operator can be constructed as
\[V = \rho_S \otimes \rho_i = \text{diag}(1, \alpha, \alpha^2, \ldots, \alpha^{N_j-1}) \otimes [(1 + \alpha)I + i(1 - \alpha)\Gamma_j \Gamma_{d+1}], \quad (S22)\]
which converts the non-Hermitian Hamiltonian in Eq. (S15) to be
\[V^{-1}H(\tilde{k})V = \frac{1}{2i}(\hat{S} - \hat{S}^\dagger) \otimes \Gamma_j - \frac{1}{2}(\hat{S} + \hat{S}^\dagger) \otimes \Gamma_{d+1} + I_{N_j} \otimes \sum_{i \neq j} \sin k_i \Gamma_i + \sqrt{M_k^2 - \lambda^2 \Gamma_{d+1}}, \quad (S23)\]
with \(M_k = M - \sum_{i \neq j} \cos M_k\).

III. BOUNDARY STATES FOR THE DIRAC MODEL WITH NON-HERMITIAN MASS TERMS

In momentum space, the lattice Dirac model with non-Hermitian mass perturbation is given by
\[H(\tilde{k}) = \sum_{i=1}^d \sin k_i \Gamma_i + (M - \sum_{i=1}^d \cos k_i)\Gamma_{d+1} + i\lambda\Gamma_{d+1}. \quad (S24)\]
The energy spectrum is \(E(\tilde{k}) = \pm \sqrt{\sum_{i=1}^d \sin^2 k_i + (M + i\lambda - \sum_{i=1}^d \cos k_i)^2}\), which is complex in general.

Taking open boundary conditions in \(j\) direction with \(N_j\) layers, the real space Hamiltonian reads,
\[H(\tilde{k}) = \frac{1}{2i}(\hat{S} - \hat{S}^\dagger) \otimes \Gamma_j - \frac{1}{2}(\hat{S} + \hat{S}^\dagger) \otimes \Gamma_{d+1} + I_{N_j} \otimes \sum_{i \neq j} \sin k_i \Gamma_i + (M - \sum_{i \neq j} \cos k_i)\Gamma_{d+1} + i\lambda \otimes \Gamma_{d+1}, \quad (S25)\]
the spectrum of which is also complex in general. Clearly, from Eqs. (S24) and (S25), the non-Hermitian mass term is equivalent to making the Hermitian mass term complex, \(M \to M + i\lambda\).

Except for \(j\) direction, the translational symmetry in other directions is preserved. We adopt the ansatz \(|\psi_k\rangle = \sum_{i=1}^{N_j} \beta_i |i\rangle \otimes |\xi_k\rangle\) with \(|\beta| < 1\) for the boundary states. In solving the Schrödinger equation, we find it gives two constraints,
\[\left[\sum_{i \neq j} \sin k_i \Gamma_i + \frac{1}{2i}(\beta - \beta^{-1})\Gamma_j + (M - \sum_{i \neq j} \cos k_i)\right] |\xi_k\rangle = \hat{E}_k |\xi_k\rangle, \quad (S26)\]
and
\[\left[\sum_{i \neq j} \sin k_i \Gamma_i + \frac{1}{2i}(\beta + \beta^{-1})\Gamma_{d+1} + i\lambda\Gamma_{d+1}\right] |\xi_k\rangle = \hat{E}_k |\xi_k\rangle. \quad (S27)\]
The difference between above two equations yields a simpler relation,
\[i\Gamma_{d+1} \Gamma_j |\xi_k\rangle = |\xi_k\rangle. \quad (S28)\]
This means the boundary states are the positive eigenvalue of \(i\Gamma_{d+1} \Gamma_j\), from which we can construct the projector for the boundary states
\[P = \frac{1}{2} (1 + i\Gamma_{d+1} \Gamma_j). \quad (S29)\]

Notice with the relation of Eq. (S28), Eq. (S27) becomes,
\[\left[\sum_{i \neq j} \sin k_i \Gamma_i + (M - \sum_{i \neq j} \cos k_i + i\lambda - \beta)\Gamma_{d+1}\right] |\xi_k\rangle = \hat{E}_k |\xi_k\rangle, \quad (S30)\]
and under the projection \(P\), Eq. (S27) also becomes,
\[\sum_{i \neq j} \sin k_i \Gamma_i |\xi_k\rangle = \hat{E}_k |\xi_k\rangle. \quad (S31)\]

The difference between above two equations gives,
\[\beta = M - \sum_{i \neq j} \cos k_i + i\lambda. \quad (S32)\]

We now calculate the effective boundary Hamiltonian. Remarkably, since the non-Hermitian mass term \(i\lambda\Gamma_{d+1}\) anti-commutes with \(i\Gamma_{d+1} \Gamma_j\) of the projector \(P\), it will vanish after the projection. Thus, the resultant effective boundary Hamiltonian is
\[H_b(\tilde{k}) = \sum_{i \neq j} \sin k_i \gamma^i, \quad (S33)\]
with \(\gamma^i = \Gamma_i \gamma P\), for \(k\) satisfying \(|\beta| = |M - \sum_{i \neq j} \cos k_i + i\lambda| < 1\). The localization region obtained this way is identical to that by the method of biorthogonal bulk-boundary correspondence [S1]. From the effective boundary Hamiltonian, boundary spectrum is purely real of \(E_b(\tilde{k}) = \pm \sqrt{\sum_{i \neq j} \sin^2 k_i}\).

[S1] F. K. Kunst, E. Edvardsson, J. C. Budich, and E. J. Bergholtz, Phys. Rev. Lett. 121, 026808 (2018).