

Absence of topological insulator phases in non-Hermitian PT -symmetric Hamiltonians

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In this work, we consider a generalization of the symmetry classification of topological insulators to non-Hermitian Hamiltonians, which satisfy a combined PT symmetry (parity and time reversal). We show via examples and explicit proofs from separate bulk and gapless boundary-state perspectives that the typical paradigm of forming topological insulator states from Dirac Hamiltonians is not compatible with the construction of non-Hermitian PT -symmetric Hamiltonians. The topological insulator states are PT -breaking phases and have energy spectra that are complex (not real) and, thus, are not consistent quantum theories.

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With recent interest generated in the field of topological insulators and superconductors,^{1–8} the symmetry classification of (primarily free-fermion) Hamiltonians has resurfaced.^{9–13} The first example of a topological insulator (TI), the integer quantum Hall effect (IQHE), is gapped in the bulk and exhibits gapless, robust states on its boundaries. Most other examples of topological insulators^{1,3–8} share these characteristic features. One interesting distinction between the IQHE and, for example, the quantum spin Hall effect (QSHE) is that the IQHE is completely robust to any type of Hamiltonian perturbation, while the QSHE is only robust to perturbations that preserve time-reversal symmetry T . A full symmetry-protected classification of topological insulators^{11,12} and superconductors¹¹ based on charge conjugation, time reversal, and chiral symmetries was then unified into a periodic table.¹³

In addition to the classification theory of TI's, Hamiltonian symmetries are important in the theory of non-Hermitian Hamiltonians,^{14–18} where it has been shown that non-Hermitian Hamiltonians can still describe viable quantum systems as long as PT symmetry is unbroken. By PT we mean the combined operation of a parity-inversion symmetry P and T . Given a non-Hermitian Hamiltonian H that satisfies $[H, PT] = 0$, one can provide necessary and sufficient conditions that the energy spectrum of H be real.¹⁶ It is thus natural to attempt to extend the periodic table of TI's to non-Hermitian Hamiltonians that satisfy PT symmetry. Although our initial hope was to find non-Hermitian examples of TI states, we instead show that TI phases are incompatible with the PT -symmetric construction of (at least a large class of) non-Hermitian Hamiltonians. The TI states are PT breaking and exhibit imaginary eigenvalues even when H has been constructed to preserve PT symmetry.

In this Brief Report, we start by showing a few pedagogical examples of PT -symmetric Dirac Hamiltonians that are perturbed away from being Hermitian. We offer these examples to show how the construction of non-Hermitian PT -symmetric TI states fails. Our focus is on Dirac Hamiltonians because they are the minimal models for topological insulators. An extension to generic insulator Hamiltonians with many bands is straightforward. After the examples, we provide more proof of necessary conditions for the bulk spectra of such Dirac Hamiltonians to have a fully real spectrum (i.e., eigenvalues are real for all values of the momenta). Finally, we give some arguments about the properties of the gapless boundary states

that show that PT symmetry, non-Hermiticity, and topological insulator states do not seem to be compatible.

Before we begin with the examples, let us list the relevant symmetry properties we will use in this Brief Report. The T operator is represented by $T = UK$, where U is a unitary operator and K is complex conjugation. Depending on U , we can have $T^2 = \pm 1$. For a Bloch Hamiltonian $H(p)$ to be invariant under T , we must have $TH(\mathbf{p})T^{-1} = H(-\mathbf{p})$. The P symmetry, which we will call *parity* when needed, is a unitary operator with $P^2 = +1$. There is no requirement on which spatial coordinates the P operator inverts, and for now we will leave it unspecified for generality. The condition that a Bloch Hamiltonian be P invariant is $PH(\mathbf{p})P^{-1} = H(\bar{\mathbf{p}})$, where $\bar{\mathbf{p}}$ is a symbol characterizing a given P by indicating which coordinates are inverted and which remain unaffected. As an example, if all the coordinates are inverted, then $\bar{\mathbf{p}} = -\mathbf{p}$. Finally, the condition that a Bloch Hamiltonian be PT symmetric is $PTH(\mathbf{p})(PT)^{-1} = H(-\bar{\mathbf{p}})$ and, equivalently, requires that $H(\mathbf{p})$ is either both odd or both even under P and T separately. We occasionally mention charge-conjugation symmetry C , which requires $CH(\mathbf{p})C^{-1} = -H^*(-\mathbf{p})$.

I. 1D DIRAC HAMILTONIANS

We will begin the examples in one dimension (1D) with the gapped continuum Dirac Hamiltonian

$$H_{1D}(p) = v_F p \sigma^y + m \sigma^z, \quad (1)$$

which is P , T , and PT symmetric with the symmetry operators $T = K$, $P = \sigma^z$, and $\bar{p} = -p$. This Hamiltonian also satisfies a C symmetry with $C = \sigma^x$ and provides an example of a Z_2 topological insulator protected by C symmetry.¹² We can add an additional term to the Hamiltonian to get

$$H'_{1D}(p) = p \sigma^y + m \sigma^z + i \Delta \sigma^x, \quad (2)$$

which is P -odd, T -odd, C -even, PT -even, and non-Hermitian, and where we set $v_F = 1$. Since we have not broken C symmetry, the Z_2 classification naively should remain intact. 1D Dirac Hamiltonians with non-Hermitian potentials have been studied, for example, in Ref. 19. The energy spectrum of this Hamiltonian is simple to calculate:

$$E_{\pm} = \pm \sqrt{p^2 + m^2 - \Delta^2}, \quad (3)$$

which is real as long as $|m| > |\Delta|$. So, we see it is possible to add a non-Hermitian perturbation to the Dirac Hamiltonian and keep the spectrum to be entirely real for values of m both <0 and >0 . Note that the perturbation has the special property $\{i\Delta\sigma^x, H_{1D}(p)\} = 0$, which will become important later.

Although it is promising that there is a regime where this non-Hermitian Hamiltonian will have a real spectrum, there is already something worrying about the spectrum. With $\Delta = 0$, this model has a gap-closing phase transition at $m = 0$, which separates a trivial insulator phase from a topological insulator phase.¹² We see here that, if $\Delta \neq 0$, this phase transition becomes destabilized when $0 < |m| < |\Delta|$. To properly describe the TI phase, we need to use a lattice version of this Dirac Hamiltonian with a Bloch form

$$H'_{1D,\text{lattice}}(p) = (\sin p)\sigma^y + (1 + m - \cos p)\sigma^z + i\Delta\sigma^x, \quad (4)$$

where we have set the lattice constant $a = 1$. When $\Delta = 0$, the lattice Hamiltonian is in a trivial insulator phase when $m < -2$ or $m > 0$, and a topological insulator phase when $-2 < m < 0$. With nonvanishing Δ , we have $E_{\pm} = \pm\sqrt{1 + (1 + m)^2 - \Delta^2 - 2(1 + m)\cos p}$. To be a viable spectrum, this must be real for all $-\pi \leq p \leq \pi$. In Fig. 1(a), we show the spectrum for $\Delta = 0$ as a function of m with open boundary conditions. This clearly shows the boundary-state zero modes, which persist when $-2 < m < 0$. In Figs. 1(b) and 1(c), we show the real and imaginary parts of the energy spectrum when $\Delta = 0.1$. This shows that, as soon as the system nears the phase boundary to the topological insulator state,

the spectrum develops imaginary pieces and thus generates a PT -breaking phase. This is a common feature and shows that the 1D topological insulator state here can not be reached when $\Delta \neq 0$.

II. 2D DIRAC HAMILTONIANS

Two dimensions (2D) become more complicated because of two reasons. (i) There are two natural definitions of P : parity $(x, y) \rightarrow (x, -y)$ and inversion $(x, y) \rightarrow (-x, -y)$, which both satisfy $P^2 = 1$. (ii) From the conventional classification theory of topological insulators, it is natural to look at both two-band and four-band models. We will not exhaust all these cases, but only provide some instructive examples.

Two-band models: Let us consider the Hamiltonian that represents the continuum model of a Chern insulator:²⁰

$$H_{2D}^{(2)}(\mathbf{p}) = p_x\sigma^x + p_y\sigma^y + m\sigma^z \quad (5)$$

with $T = K$ and $P = \sigma^x$. This P corresponds to a parity symmetry and sends $p_y \rightarrow -p_y$, so $\bar{\mathbf{p}} = (p_x, -p_y)$. Unfortunately, this Hamiltonian can not be made PT symmetric even before we perturb it because the mass term breaks PT . Next, let us consider the same Hamiltonian with $T = K$ and $P = \sigma^z$, where this P is an inversion symmetry with $\bar{\mathbf{p}} = -\mathbf{p}$. Again, even the base Hamiltonian is not PT symmetric because the p_x term breaks PT . Finally, if we consider the same Hamiltonian with $T = i\sigma^y K$ and $P = \sigma^z$ and $\bar{\mathbf{p}} = -\mathbf{p}$, the mass term breaks PT . From these few attempts, it seems like we can not get any interesting non-Hermitian TI Hamiltonians with two bands. We will see why this is so in the general proof section, but the basic idea is that there are no additional matrices M that anticommute with $H_{2D}^{(2)}(\mathbf{p})$.

Four-band models: Let us start with a continuum QSH Hamiltonian^{1,3}

$$H_{2D}^{(4)}(\mathbf{p}) = p_x\Gamma^1 + p_y\Gamma^2 + m\Gamma^0 \quad (6)$$

with $\Gamma^1 = \tau^x \otimes \sigma^x$, $\Gamma^2 = \tau^x \otimes \sigma^y$, $\Gamma^3 = \tau^y \otimes \mathbb{I}$, $\Gamma^4 = \tau^x \otimes \sigma^z$, and $\Gamma^0 = \tau^z \otimes \mathbb{I}$. This has symmetry generators $T = i\sigma^y K$ and $P = \Gamma^0$ and $\bar{\mathbf{p}} = -\mathbf{p}$. We can perturb this Hamiltonian with the non-Hermitian PT -symmetric matrices $\{i\tau^x \otimes \mathbb{I}, i\tau^y \otimes \sigma^i, i\tau^z \otimes \sigma^i, i\mathbb{I} \otimes \sigma^i\}$, but none of these anticommute with the Hamiltonian and will lead to imaginary bulk eigenvalues as we will see in the following section.

We can write down another Hamiltonian in 2D:

$$H_{2DB}^{(4)}(p) = p_x\Gamma^2 + p_y\Gamma^3 + m\Gamma^0. \quad (7)$$

This has symmetry operators $T = K$ and $P = \Gamma^0$ with $\bar{\mathbf{p}} = -\mathbf{p}$. There are two interesting terms with which we can perturb the Hamiltonian:

$$\Delta H_{2D}^{(4)} = i\Delta_1\Gamma^1 + i\Delta_4\Gamma^4. \quad (8)$$

Adding these terms to the Hamiltonian gives us an energy spectrum

$$E_{\pm} = \pm\sqrt{p_x^2 + p_y^2 + m^2 - \Delta_1^2 - \Delta_4^2}, \quad (9)$$

which is real as long as $m^2 \geq \Delta_3^2 + \Delta_4^2$. However, this model with $T = K$ is not known to exhibit a robust topological insulator state anyway, but we see that there is the same

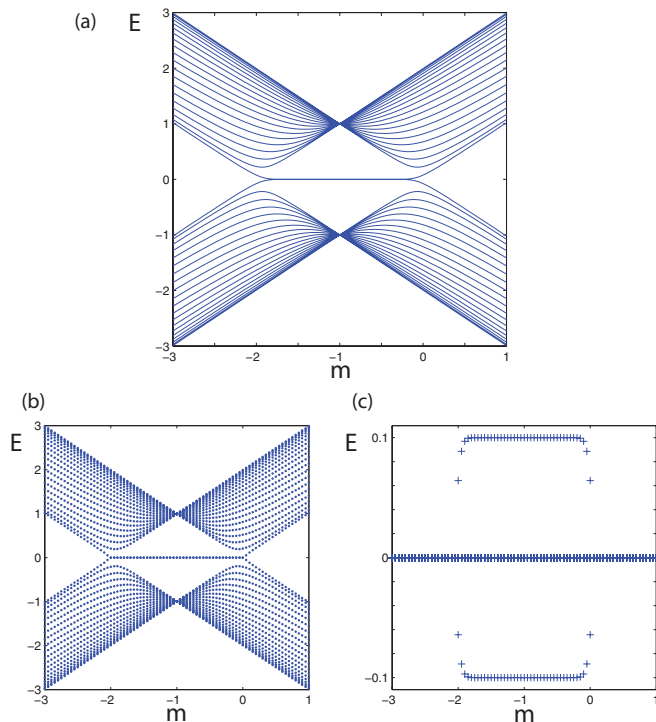


FIG. 1. (Color online) Energy spectrum of $H'_{1D,\text{lattice}}$ [Eq. (4)] with open boundaries vs m . (a) $\Delta = 0$ gives a real spectrum with zero modes for $-2 < m < 0$. (b) Real part of energy spectrum and (c) imaginary part of energy spectrum for $\Delta = 0.1$. Complex eigenvalues exist in the former topological phase.

problem with the gap-closing transition leading to a PT -breaking region.

III. NECESSARY CONDITIONS FOR REAL BULK EIGENVALUES

The generic features of the example models are that if there is a PT -symmetric, non-Hermitian matrix that anticommutes with $H(p)$, then we can have real eigenvalues, but the topological insulator phase is PT breaking. If the only PT -symmetric non-Hermitian matrices commute with at least one term of $H(p)$, then even the bulk eigenvalues will not be real for all of momentum space. We formalize this statement now.

Theorem. For a PT -symmetric Hamiltonian of the Dirac form $H = p\Gamma + mQ + i\Delta S$, where p, m, Δ are real parameters, S, Q, Γ are Hermitian (linear) matrices with $S^2 = Q^2 = \Gamma^2 = 1$ and $\{Q, \Gamma\} = 0$, the quantities $\{Q, S\}$ and $\{\Gamma, S\}$ must vanish to have a real bulk spectrum.

Proof. Assume we have a Hamiltonian

$$H(p) = p\Gamma + mQ + i\Delta S. \quad (10)$$

By contradiction, let us assume that $[S, Q] = 0$ so that the anti-Hermitian term commutes with the mass term. For the point $p = 0$, the Hamiltonian reduces to $H(0) = mQ + i\Delta S$. Since S and Q commute, they can be simultaneously diagonalized. Since $S^2 = Q^2 = +1$, the eigenvalues of these matrices are ± 1 . Thus, the eigenvalues of $H(0)$ can only be $\pm m \pm i\Delta$ and are always imaginary if $\Delta \neq 0$. This is a contradiction and so we know that $\{S, Q\} = 0$ must hold if the spectrum is to be real for all allowed p .

Now, we want to prove the second necessary condition by contradiction. Assume that $\{S, Q\} = 0$, which we now know must hold, but $[S, \Gamma] = 0$. The Hamiltonian at finite p is as above and $H^2(p) = (p^2 + m^2 - \Delta^2)\mathbb{I} + ip\Delta\{\Gamma, S\}$. From our assumptions $\{\Gamma, S\} = 2\Gamma S$ and $(\Gamma S)^2 = +1$, so the eigenvalues of $\{\Gamma, S\}$ are ± 1 . Thus, the eigenvalues of $H^2(p)$ are

$$E_{\pm}^2 = (p^2 + m^2 - \Delta^2) \pm 2ip\Delta \\ \Rightarrow \pm E_{\pm} = \pm \sqrt{(p \pm i\Delta)^2 + m^2}. \quad (11)$$

This means that, for all nonzero p , the eigenvalues will be imaginary. This is a contradiction and thus we have proven that both $\{S, Q\} = \{S, \Gamma\} = 0$ are necessary conditions for the bulk spectra to be real. ■

Corollary. For Hamiltonians of the form $H(p) = p_a\Gamma^a + mQ + i\Delta S$, where $\{\Gamma^a, Q\} = 0$ and $(\Gamma^a)^2 = Q^2 = S^2 = 1$, we must have $\{S, \Gamma^a\} = \{S, Q\} = 0$ for all values of a .

Proof. The case involving the mass term is unchanged from above. For the momentum term, by contradiction, assume that there is a value $a = a_0$ such that $[S, \Gamma^{a_0}] = 0$. We can then set all $p_a = 0$ for $a \neq a_0$ and use the same theorem as above to prove the result. ■

Thus, we see that, to give a real spectrum, we must have an S that is a Clifford algebra generator along with the generators Γ^a and Q . To satisfy PT symmetry, we need

$$(PT)iS(PT)^{-1} = -i(PU)S^*U^{-1}P^{-1} = iS \\ \Rightarrow (PU)S^* + S(PU) = 0; \quad (12)$$

this means that, if $S = S^*$, then PT symmetry requires $\{PU, S\} = 0$. If $S = -S^*$, then PT symmetry requires $[PU, S] = 0$. The form of the energy spectrum for such an anticommuting S will be $E_{\pm} = \pm \sqrt{\sum_a p_a^2 + m^2 - \Delta^2}$.

IV. BOUNDARY AND INTERFACE STATES

Let us return back to the 1D Hamiltonian specified in Eqs. (1) and (2). There is a region of the TI phase (i.e., where $-2 < m < 0$) where $|m|$ could be greater than $|\Delta|$ and thus could have a real bulk spectrum, but from Figs. 1(b) and 1(c), we see that the phase is still PT breaking. To illustrate why the TI state is PT breaking, we need to consider the gapless boundary states. We will do this in the simplest possible way and capture the essential details by considering two interfaces between regions described by Dirac Hamiltonians with $m(x) = -m_0$ for $x < -x_0$ next to a region with $m(x) = m_0 > 0$ for $-x_0 < x < x_0$, and, finally, with $m(x) = -m_0$ for $x > x_0$. We assume that $|m_0| \geq |\Delta|$ so that the bulk energy spectrum is real in each region, and that $2x_0 \gg \hbar v_F/m_0$ so that, for our purposes, the interfaces are independent of each other. Note that this potential satisfies $m(x) = m^*(-x)$ and is thus PT symmetric. The 1D Hamiltonian is

$$H = -i \frac{d}{dx} \sigma^y + m(x) \sigma^z. \quad (13)$$

This Hamiltonian has two zero-energy bound states,²¹ one per interface domain wall given by

$$\Psi_0^{\pm}(x) = \frac{1}{\sqrt{2}} \exp \left[\pm \int_{\pm x_0}^x m(x') dx' \right] \begin{pmatrix} 1 \\ \mp 1 \end{pmatrix}. \quad (14)$$

We see something interesting that occurs here:

$$PT\Psi_0^+(x) = P\Psi_0^{+*}(x) = \sigma^z\Psi_0^{+*}(-x) = \Psi_0^-(x). \quad (15)$$

This means that Ψ_0 is not an eigenstate of PT and, thus, we do not expect it to have a real eigenvalue if we add a non-Hermitian PT -symmetric term.^{15,16} The PT symmetry transforms one boundary state into the other one. This is not so strange since the P symmetry should interchange the two ends of the 1D system, or in this case the states on each domain wall.

Now, let us perturb the Hamiltonian by $i\Delta\sigma^x$, as in the 1D example above, and focus near a single domain wall. The unperturbed system has Ψ_0 as a zero-energy state. Adding the perturbation is trivial since Ψ_0 is *already* an eigenstate of σ^x . Thus, we see that perturbing the domain-wall states changes the energies of the states from $E = 0$ to $\pm i\Delta$, which is obviously imaginary. Thus, the domain wall, and by analogy, TI boundary states, break the PT symmetry and are not compatible with a real energy spectrum.

To show that this is not a pathological case for the 1D Hamiltonian, let us consider the 2D Hamiltonian in Eq. (7), which will still have (unprotected) bound states on mass domain walls. We will assume the domain walls are in the y direction this time. The Hamiltonian is then

$$H_{2D}^{(4)} = p_x \Gamma^2 - i \frac{d}{dy} \Gamma^3 + m(y) \Gamma^0, \quad (16)$$

where p_x is a number. For $p_x = 0$, we can use the same ansatz as in the 1D case, but this time there are two zero-energy

solutions per wall. For an upward-stepping domain wall, we find

$$\Psi_{0A} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}, \quad \Psi_{0B} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}. \quad (17)$$

For $p_x \neq 0$, these solutions *do not* automatically diagonalize Γ^1 and we are left with a reduced 2×2 problem

$$H_{ij}^{(\text{eff})} = \langle \Psi_{0i} | p_x \Gamma^2 | \Psi_{0j} \rangle = p_x \sigma_{ij}^y, \quad (18)$$

where $i, j = A, B$. Now, if we add the allowed, anticommuting non-Hermitian terms $i\Delta_1\Gamma^1 + i\Delta_4\Gamma^4$, the effective Hamiltonian of the edge states becomes

$$\begin{aligned} H_{ij}^{(\text{eff})} &= p_x \sigma_{ij}^y + \langle \Psi_{0i} | i\Delta_1\Gamma^1 + i\Delta_4\Gamma^4 | \Psi_{0j} \rangle \\ &= p_x \sigma_{ij}^y + i\Delta_1 \sigma_{ij}^x + i\Delta_4 \sigma_{ij}^z. \end{aligned} \quad (19)$$

This Hamiltonian is simple to diagonalize and has energies

$$E_{\pm} = \pm \sqrt{p_x^2 - \Delta_1^2 - \Delta_4^2}, \quad (20)$$

which are imaginary at least at $p_x = 0$ if either of the $\Delta_i \neq 0$. Thus, again the boundary spectrum is imaginary. The states $\Psi_{0A/B}$ are not eigenstates of the PT operator and will be transformed into the allowed states on the opposite wall by PT . These arguments generalize to the other topological insulator classes and show that such a phase is always PT breaking.

With this proof in place, one can immediately begin to search for exceptions. The first place to look would be topological superconductors, the boundary states of which have weight on both boundaries. We performed a cursory test of some classes of topological superconductors and were not able to construct an interesting non-Hermitian PT -symmetric phase. The presence of Majorana boundary fermions, which are nonlocal, may provide a way around the boundary state problem, but we leave this open for future work. Also, our result does not immediately apply to topological insulator states protected by point-group symmetries such as inversion^{22–24} or even $C4$ symmetry.²⁵ In this case, however, we believe that our result can easily be adapted to at least a large class of these models since again they can usually be expressed using minimal Dirac-type models where our results would immediately carry over. This does leave open the possibility of finding non-Hermitian topological phases, but without Dirac-type Hamiltonians at their foundation.

Recently, a preprint appeared with overlapping results.²⁶ Where the papers overlap, the results agree. The motivation behind the two works is quite different and our interpretation of the appearance of complex energy eigenvalues as an inconsistency in the quantum theory is strict compared to that work.

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