Non-Abelian Berry Gauge Field and Topological Invariant in Parity-Time Symmetric Non-Hermitian Spin-1/2 Quantum Systems

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Recently developed parity \((\mathcal{P})\) and time-reversal \((\mathcal{T})\) symmetric non-Hermitian quantum theory is envisioned to have far-reaching implications and applications. It is known that the \(\mathcal{P}\mathcal{T}\)-inner product is defined with respect to a non-canonical, system generated symmetry, namely the \(\mathcal{C}\) symmetry. We show that the \(\mathcal{P}\mathcal{T}\) symmetric equation of motion is defined by the simultaneous time evolution of the state \(\psi(t)\) and the operator \(\mathcal{C}(t)\) manifesting unitarity – a situation analogous to the Dirac/interaction picture. The time-dependent \(\mathcal{C}\) operator lends itself into a new term in the Berry phase, setting a platform for novel and exotic topological phases. We also point out that the gauge invariance is achieved by a more generic \(\mathcal{C}\mathcal{P}\mathcal{T}\) gauge transformation, not by the usual unitary gauge transformation. The \(\mathcal{P}\mathcal{T}\) symmetric theory is not generally applicable for spin-1/2 fermions, since here \(\mathcal{P}\mathcal{T}\) inner product becomes undefined due to Kramer’s theory. We propose a realizable non-Hermitian setup for spin-1/2 fermions which acquires the combined \(\mathcal{P}\mathcal{T}\)^2 = +1 symmetry, despite \(\mathcal{T}^2 = -1\) and \(\mathcal{P}^2 = +1\). The Hamiltonian inherits non-Abelian Berry gauge fields for non-interacting fermions without magnetic field. The corresponding edge states are found to have unique supersymmetric oscillator solutions but with complex energy levels.

Non-Abelian Berry gauge field and corresponding topological phases can arise in degenerate ground states with non-trivial band structure.\(^{1-5}\) Such systems are highly desirable for obtaining anyons, fractons, supersymmetry with their implications for quantum computing and other applications.\(^{6-11}\) The fractional quantum Hall states with applied magnetic field (mainly \(\nu = 5/2\) state)\(^{12-15}\) or certain interacting topological antiferromagnetic insulators\(^{4-5,16}\), and topological superconductors\(^{17,18}\) provide viable routes to obtain non-Abelian excitations in condensed matter setup. However, proposals and realizations of intrinsic generation of non-Abelian states in non-interacting systems and without applied magnetic field are long-sought in condensed matter and materials science community.

Topological phases in non-Hermitian (NH) Hamiltonians without and with real energy have been widely explored in recent years.\(^{19}\) Owing to complex energy spectrum and biorthogonal probability density, one may expect a plethora of distinct topological invariants in NH systems which may or may not have any direct analogue with their Hermitian counterparts.\(^{20,21}\) Such studies can become more interesting in NH systems which posses real eigenenergies and conserved probability density with the help of pseudo-Hermitian metric.\(^{22}\) and/or parity \((\mathcal{P})\) - time reversal \((\mathcal{T})\) symmetry invariance.\(^{23}\) So far Abelian topological phases are mainly studied in various NH systems.\(^{20-21,24}\) Band degeneracy, a prerequisite for non-Abelian phases, is quite exceptional in NH systems, since here the corresponding wavefunctions coalesce.\(^{25}\) Such exceptional points apparently hinder the possibility to stabilizing non-Abelian phases in this class of materials.

Our work presents several novel features. (i) While \(\mathcal{P}\mathcal{T}\) symmetry solely can guarantee real eigenvalues, the \(\mathcal{P}\mathcal{T}\)-inner product is not always positive, definite.\(^{23}\) Moreover, the time-evolution of the state is not always ‘unitary’. This is remedied by defining a hidden, non-canonical symmetry, often termed as \(\mathcal{C}\) symmetry, such that the \(\mathcal{C}\mathcal{P}\mathcal{T}\)-inner product is positive definite.\(^{23}\) Intriguingly, we show that the conservation of the probability density is defined by the simultaneous time-evolution of state \(\psi(t)\) and the \(\mathcal{C}(t)\) operator. This situation is reminiscence of the Dirac/interaction picture, except here physical operators are not necessarily time-dependent. (ii) We also find that adiabatic time evolution of both \(\psi(t)\), \(\mathcal{C}(t)\) conspires a new and important term to the Berry phase and topological invariants. (iii) Interestingly, the \(U(N)\) gauge invariance and co-variance of the Berry phase and Berry connection, respectively, are defined with respect to a \(\mathcal{C}\mathcal{P}\mathcal{T}\) invariant gauge transformation, replacing the usual unitary transformation for the Hermitian counterparts. (iv) The above \(\mathcal{P}\mathcal{T}\)-invariant quantum theory is generally defined for \((\mathcal{P}\mathcal{T})^2 = 1\), in which case the Hamiltonian and \(\mathcal{P}\mathcal{T}\) operator share the same eigenfunctions. For spinful systems, this is generally a problem since here \(\mathcal{T}^2 = -1\), making the \(\mathcal{P}\mathcal{T}\)-inner product to vanish for all eigenstates (Kramer’s degeneracy). To bypass this problem, we propose a setup with coupled quantum wires with opposite NH spin-orbit coupling (SOC) in adjacent layers. The setup is designed to possess ‘parity’ \(\mathcal{P}\) via spin and sublattice inversions, such that \(\mathcal{P}\) and \(\mathcal{T}\) anticommutes with each other, giving \((\mathcal{P}\mathcal{T})^2 = +1\), despite \(\mathcal{P}^2 = +1\), and \(\mathcal{T}^2 = -1\). The system possesses real eigenvalues, and conserved \(\mathcal{C}\mathcal{P}\mathcal{T}\) inner product under a dynamical \(\mathcal{C}\) operator. (v) Under the \(\mathcal{C}\mathcal{P}\mathcal{T}\) invariance, the system possess degeneracy which intrinsically governs non-Abelian Berry connection, and winding number in a periodic boundary condition. (vi) Finally, we show that the edge state of the non-trivial topological phase has unique solutions. Two edge states are found to possess coupled harmonic oscillator like solutions, with complex but quantized eigenvalues and localized Gaussian wavepackets. More intriguingly, the two solutions are related to each other by mutually skipping eigenstates – a situation which is qualitatively analogous to the ‘supersymmetric’ oscillator solutions,\(^{20}\) but generalized here for com-
complex energies.

**Non-Abelian Berry matrix in CPT - theory.** Let $H$ be a generic $\mathcal{PT}$ - invariant Hamiltonian defined as $H = (\mathcal{PT}) H^T (\mathcal{PT})^{-1}$, where $T$ is the transpose operation. The following discussions hold for this generic requirement, however, as often done, we specialize henceforth to the symmetric ($H^T = H$) Hamiltonians. This implies that the specific $\mathcal{PT}$ - invariance is defined by the commutator $[H, \mathcal{PT}] = 0$.\[23\]

The Hamiltonian follows the eigenvalue equation: $H |\psi_n\rangle = E_n |\psi_n\rangle$, where eigenvalues $E_n$ are real due to $\mathcal{PT}$ invariance. An essential generic issue of the $\mathcal{PT}$-invariant quantum theory is that the $\mathcal{PT}$-inner product is not a constant of motion, and hence there exists a *dynamical*, and non-canonical symmetry $\mathcal{C}$ which evolves in time in such a way that the $\mathcal{PT}$ - inner product becomes conserved. The operator follows $[H, \mathcal{C}] = 0$, and $[\mathcal{PT}, \mathcal{C}] = 0$, with the $\mathcal{PT}$-inner product defined as $\langle \psi^\mathcal{PT}_m | \psi_n \rangle \equiv \langle \psi^\mathcal{PT}_m | \mathcal{C} \mathcal{PT} | \psi_n \rangle = \int d^dx (\mathcal{C} \mathcal{PT} | \psi_m \rangle)^T \mathcal{C} | \psi_n \rangle = \delta_{mn}$.\[\]

For a Hermitian case, the time evolution of the state is solely governed by the Hamiltonian itself. This is not generally true for NH systems. Let $Q$ be a linear time evolution operator for the eigenstates satisfying $i \hbar \dot{|\psi_n\rangle} = Q |\psi_n\rangle$. The conservation of the $\mathcal{PT}$ - inner product dictates the equation of motion to be $i \hbar \dot{\psi}^\mathcal{PT} = [Q, \mathcal{PT}] |\psi_n\rangle$.\[27\] Interestingly, $Q$ is not $\mathcal{PT}$ - invariant, in general, otherwise, $\mathcal{C}$ operator becomes a constant of motion. Equating for the $Q$ operator to be $Q = H + |\hbar|^2/2 \mathcal{C}^{-1} \mathcal{C}$, we obtain the equation of motion of the eigenstates as

$$i \hbar \dot{|\psi_n\rangle} = H |\psi_n\rangle + \frac{i \hbar}{2} \mathcal{C}^{-1} |\psi_n\rangle.$$\(\text{(1)}\)

(As mentioned in the introduction, both the state and the $\mathcal{C}$ operator evolves in time – somewhat analogous to the Dirac/interaction picture, however, here other operators do not necessarily evolve in time.)

Next, we consider that the eigenstates $|\psi_n\rangle$ are $N$-fold degenerate. The solution of Eq. (1) for such a degenerate ground state in an adiabatic path yields a solution which evolves as $|\psi_n\rangle \rightarrow \sum_m |\psi_m\rangle Y_{mn}$. $\Gamma$ is the $N \times N$ Berry rotational matrix $\Gamma = e^{i\gamma}$, and $\gamma$ is the $N \times N$ Berry phase matrix, defined as

$$\gamma = \int A_\mu dx^\mu,$$\(\text{(2)}\)

where $\mu$ index runs over the spatial dimensions of the system (in position or momentum space in which the Hamiltonian is considered). $A$ is the non-Abelian Berry connection matrix obtained to be \[27\]

$$A_{\mu, mn} = i \langle \psi_m | CPT | \partial_\mu \psi_n \rangle - i \frac{1}{2} \langle \psi_m | (\partial_\mu C) \mathcal{PT} | \psi_n \rangle.$$\(\text{(3)}\)

where $m, n$ indices run over the $N$ fold degenerate eigenstates. Notice that the second term is a new contribution arising from the adiabatic evolution of the dynamical operator $C$.

How does the Berry connection transform under the $U(N)$ gauge transformation, and how is the corresponding gauge co-variance defined? To find it out, let $|\psi'_n\rangle$ be a different choice of the eigenstate which is rotated by a $U(N)$ gauge as: $|\psi'_n\rangle = \sum_m |\psi_m\rangle U_{mn}$. Given that the inner product must be invariant under a $U(N)$ gauge transformation, i.e., $\langle \psi'_m | \mathcal{PT} | \psi'_n \rangle = \langle \psi_m | \mathcal{PT} | \psi_n \rangle$, we obtain the crucial property\[27\]:

$$(U^T)^{\mathcal{PT}} U = 1,$$\(\text{(4)}\)

where $1$ is the $N \times N$ identity matrix.\[23\] Eq. (4) is the replacement of the unitary condition for $U(N)$ in the Hermitian case. If $A'_\mu$ is the Berry connection in the new basis, then we have the $U(N)$ gauge co-variance defined by (in matrix form):

$$A'_\mu = (U^T)^{\mathcal{PT}} [A_\mu + i \partial_\mu] U.$$\(\text{(5)}\)

All the observables ($O$), such as Berry curvature, Berry rotation matrix $\Gamma$, transform under the $\mathcal{PT}$ - invariant $U(N)$ gauge transformation as $O' = (U^T)^{\mathcal{PT}} O U$. Consequently, we can define the winding number matrix as $w_{mn} = \gamma_{mn}/2\pi$ in odd dimensions, and the Chern matrix as the flux of the corresponding Berry curvature in a periodic boundary condition in even dimensions.

**The Hamiltonian.** Inspired by the fact that $\mathcal{PT}$-symmetric systems can be readily engineered in optical lattices,\[21\] and that SOC is also realized in 1D optical lattices,\[29\] we construct a setup made of coupled 1D optical wires with NH SOC.
Here we achieve non-Hermiticity in the SOC term, with anti-Hermitian SOC term between $\uparrow\leftrightarrow\downarrow$, as shown in Fig. 1(a). The corresponding NH Hamiltonian for a single 1D wire is defined as $h_k = \epsilon_k \sigma_0 + i \alpha_k \sigma_z$, where $\epsilon_\alpha$ are the $2 \times 2$ Pauli matrices and $\sigma_0$ is a unit matrix. The band dispersion $(\epsilon_k)$, and SOC amplitude ($\alpha_k$) are real. This Hamiltonian breaks $\mathcal{PT}$ symmetry as evident from its complex eigenvalues $\xi_{k,\pm} = \epsilon_k + i \alpha_k$. The corresponding right eigenvectors are $|\psi_{k,\pm}^R\rangle = 1/\sqrt{2}(1, \pm 1)^T$. The NH Hamiltonian $h_k$ also has a corresponding left counterpart $h_k^\dagger$, with left eigenvectors $\langle \psi_{k,\pm}^L | = (\psi_{k,\pm}^R)^T$, and left eigenvalues $\xi_{k,\pm}^*$, as shown in Fig. 1(b).

The trick we propose here is to quantum mechanically couple two adjacent 1D SOC wires to act as the right and left counterparts to each layer, as shown in Fig. 1(c). The adjacent layers are coupled by quantum tunneling amplitude $b_{k\sigma}$. The full setup is thus defined in a four-component spinor $\psi_k = (\psi_{k,\uparrow}^R, \psi_{k,\uparrow}^L, \psi_{k,\downarrow}^L, \psi_{k,\downarrow}^L)$ as

$$H_k = \begin{pmatrix} h_k & V_k \\ V_k^\dagger & h_k^\dagger \end{pmatrix},$$

(6)

where $V_k = \text{diag}(b_{k\uparrow}, b_{k\downarrow})$.

Eigen spectrum. The eigenvalues of Eq. (6) are

$$E_{1,3} = \epsilon \pm (b_+ - b_-), \quad E_{2,4} = \epsilon \pm (b_+ + b_-),$$

(7)

where $k$-dependence is suppressed for simplicity. $b_{k\uparrow} = \frac{1}{2}(b_{k\uparrow} + b_{k\downarrow})$ and $b_{k\downarrow} = \sqrt{(b_{k\uparrow})^2 - \alpha_k^2}$. Since $\epsilon_k$ and $\alpha_k$ are always real, the $\mathcal{PT}$-invariant region is simply defined by the region where $|b_{k\uparrow}|$ is real, i.e., $|b_{k\uparrow}| > |\alpha_k|$, as shown in Fig. 2(lower panel). The following calculations and presentations become transparent in the complex polar coordinate defined by $b_{k\uparrow} = \xi_{k\uparrow} \cosh \theta_k$, and $\alpha_k = \xi_{k\downarrow} \sinh \theta_k$. The corresponding eigenvectors are

$$\psi_{1,3} = \frac{1}{\sqrt{2}} \begin{pmatrix} \sinh \frac{\theta}{2} \\ \pm \cosh \frac{\theta}{2} \\ \pm \sinh \frac{\theta}{2} \\ -\cosh \frac{\theta}{2} \end{pmatrix}, \quad \psi_{2,4} = \frac{1}{\sqrt{2}} \begin{pmatrix} -i \cosh \frac{\theta}{2} \\ \mp \sinh \frac{\theta}{2} \\ \mp i \cosh \frac{\theta}{2} \\ \sinh \frac{\theta}{2} \end{pmatrix}$$

(8)

(k dependence is implicit). Evidently, eigenvectors do not depend on $b_{k\downarrow}$ and $\epsilon_k$, and hence play no role on the topology. The SOC amplitude is odd under inversion, so the minimal dispersion it obtains is $\alpha_k = \alpha_0 \sin k$ where $\alpha_0$ is real. Finally, the hopping between ‘R’ and ‘L’ wires is $b_{k\sigma} = b_{k\sigma} + b_{k\sigma} \cos k$, where $\sigma = \uparrow / \downarrow$, and $b_{k\sigma}$ are real parameters.

Symmetry properties. Its now worthwhile delineating the symmetry properties of the Hamiltonian. In a NH, $\mathcal{PT}$-symmetric Hamiltonian, $(\mathcal{PT})^2 = +1$ is generally a requirement to ensure real eigenvalues. But for half-integer spin, we have $\mathcal{T}^2 = -1$, and $\mathcal{P}^2 = +1$, so that $\langle \psi_n | \mathcal{PT} | \psi_n \rangle = 0$ for all $n$ states, and hence the $\mathcal{PT}$ conjugate Hilbert space collapses. We succeed overcoming this challenge by the special design of the setup, in which the two adjacent wires not only act as right and left eigenstates, but also serve as $\mathcal{PT}$ conjugate to each other.

In our Hamiltonian, both coefficients $i \alpha_k$ and $b_{k\sigma}$ break $\mathcal{T}$ symmetry; with $i \alpha_k$ is $\mathcal{PT}$ invariant, while $b_{k\sigma}$ is not (since $b_{k\sigma}$ is even under spatial inversion). This implies that the $\mathcal{P}$ operator cannot be a simple chiral inversion (i.e., $R \leftrightarrow L$), but must also involve spin inversion and at the same time be unitary. Hence the total ‘parity’ operator is a combination of momentum and spin inversions: $\mathcal{P} = \tau_y \otimes \sigma_z$, with $\mathcal{P}^2 = +1$. ($\tau_y$ are Pauli matrices defined in the chiral basis with $\tau_0$ is unit matrix.) The TR operator consists of momentum inversion and spin flips: $\mathcal{T} = i \tau_0 \otimes \sigma_y \mathcal{K}$, with $\mathcal{T}^2 = -1$ and $\mathcal{K}$ is the complex conjugation operator. Since $\{ \mathcal{T}, \mathcal{P} \} = 0$, we achieve $(\mathcal{PT})^2 = +1$.

For this $\mathcal{PT}$-operator, the $\mathcal{PT}$ inner product of the eigenstates of Eq. (6) gives $\langle \psi_m | \mathcal{PT} | \psi_n \rangle = (-1)^n \delta_{mn}$. Therefore, to achieve positive, definite inner product, we define a $\mathcal{C}$ operator as $\mathcal{C} = \sum_n \langle \psi_n | \mathcal{PT} | \psi_n \rangle$, which gives

$$\mathcal{C}_k = (\tau_0 \otimes \sigma_z) \cosh \theta_k + i (\tau_y \otimes \sigma_y) \sinh \theta_k.$$  

(9)

This gives $\langle \psi_m | \mathcal{C}_k \mathcal{PT} | \psi_n \rangle = \delta_{mn}$, in which the $k$ dependence of the $\mathcal{C}_k$ operator plays a crucial role.

In addition, the Hamiltonian in Eq. (6) has both the charge conjugation $\mathcal{Y}$ and chiral $\Xi$ symmetries. We find that $\mathcal{Y} = \tau_z \otimes \sigma_0 \mathcal{K}$, and $\Xi = \mathcal{Y} \mathcal{PT}$. Under these symmetries the Hamiltonian transforms as $\mathcal{Y} H_k \mathcal{Y}^{-1} = - H_{-k}$, and $\Xi H_k \Xi^{-1} = - H_k$. Both symmetries give particle-hole symmetric spec-
trum \pm E_n (n is the band index). In our case, such a condition is satisfied if the Hamiltonian is traceless, i.e. $\epsilon_k = 0$ at all k-points.

**Non-Abelian Berry phase.** There exist some intriguing relationships between the odd and even eigenstates of Eq. (3).

(i) We have $\partial_k \psi_{1,3} = i \frac{\partial k}{\partial k} \psi_{2,4}$, and vice versa. (ii) Furthermore, $\psi_{1,3}$ and $\psi_{2,4}$ are related to each other by a rotation of $\pi/2$ and a phase of $\pi/2$. These redundancies suggest that there exists an inherent ground state degeneracy in this system. These two conditions guarantee the existence of a robust non-Abelian Berry phase between $\psi_1 \leftrightarrow \psi_2$, and $\psi_3 \leftrightarrow \psi_4$ under adiabatic evolution of the state. Furthermore, with a periodic boundary condition, the corresponding winding numbers are quantized.

The Berry connection from Eq. (3) have two terms. The adiabatic evolution of the eigenstate yields the first term: $A_{mn}^{\alpha} = i \langle \psi_m | \mathcal{C}_k \mathcal{P} \mathcal{T} | \psi_n \rangle = -i \frac{\partial k}{\partial k} (\tau_0 \otimes \sigma_x)_{mn}$. The same evolution of the $\mathcal{C}_k$ operator gives $A_{mn}^{\alpha} = -\frac{i}{2} \langle \psi_m | (\partial_k \mathcal{C}_k) \mathcal{P} \mathcal{T} | \psi_n \rangle = A_{mn}^{\alpha}$. Hence the total Berry connection (matrix) is

$$A = -\partial_k \theta_k (\tau_0 \otimes \sigma_x).$$

Clearly, the Berry connection is purely non-Abelian (off-diagonal), and does not have any Abelian (diagonal) component.

The corresponding Berry matrix is $\gamma = (\tau_0 \otimes \sigma_x) \otimes \partial_k \theta_k$. Here, we point out an interesting feature of the angle $\theta_k = \tanh^{-1} (\frac{\alpha_k}{\alpha_{k+}})$. The $\mathcal{PT}$-symmetric region is defined by $\alpha_k/\alpha_{k+} \leq 1$, rendering $\theta_k \rightarrow \infty$ at the $\mathcal{PT}$-symmetric boundary, and finite inside.

In Fig. 2, we examine the topological phase diagram in three representative regions. In the $\mathcal{PT}$-symmetric region, $|\alpha_k| \leq |\alpha_{k+}|$ condition opens a band gap across the Fermi level. For $b_{k+} = b_k$, there is a two-fold degeneracy at all k-points. $b_{k+} \neq b_k$ lifts the degeneracy except at characteristic k-points where bands are inverted. The existence of these characteristic band inversion k-points within the Brillouin zone is responsible for finite non-Abelian Berry phase in the setup. Finally, in the $\mathcal{PT}$-broken region for $|\alpha_k| > |\alpha_{k+}|$, see Figs. 2c,f, we find that the non-Abelian Berry phase persists but becomes a complex number.

**Boundary states.** The bulk-boundary correspondence for the $\mathcal{PT}$-symmetric NH topological insulator is not as concrete as in the Hermitian case. This is because even when the $\mathcal{PT}$-symmetry is intact in the bulk, this symmetry may be lost at the boundary for the same parameter region. In our model, the $\mathcal{PT}$ symmetry is broken at the boundary giving complex energy. However, interestingly, the boundary states are localized at the edge like a harmonic oscillator.

For the discussion of the boundary state, a suitable choice of basis is:

$$\phi_{k+} = \frac{1}{\sqrt{2}} (\psi_{k+}^R + i \psi_{k+}^L),$$
$$\phi_{k-} = \frac{1}{\sqrt{2}} (\psi_{k+}^R - i \psi_{k+}^L),$$
$$\phi_{k+} = \frac{1}{\sqrt{2}} (\psi_{k+}^R + i \psi_{k+}^L),$$
$$\chi_{k+} = \frac{1}{\sqrt{2}} (\psi_{k+}^R - i \psi_{k+}^L).$$

The rotated Hamiltonian in this basis acquires a simpler block diagonal form with two degenerate blocks for $b_{k-} = 0$ (recall that $b_{k-}$ does not contribute to the eigenstates, and hence topology remains intact). Hence we can seek solutions of each $2 \times 2$ Block Hamiltonian which follows

$$i \begin{pmatrix} 0 & b_{k+} + \alpha_k \\ -b_{k+} + \alpha_k & 0 \end{pmatrix} \begin{pmatrix} \phi_k \\ \chi_k \end{pmatrix} = E_k \begin{pmatrix} \phi_k \\ \chi_k \end{pmatrix}. \tag{12}$$

(We drop the subscript $\pm$ in the states for simplicity.) We solve Eq. (12) with the open boundary conditions for edge state solutions. In the long-wavelength limit, the SOC term gives $\alpha_k \rightarrow i \alpha_0 \partial/k \partial x$ (we set $\hbar = 1$) and $b_{k+}$ gives the domain wall potential as $b_0 x$ ($\alpha_0$ and $b_0$ are real constants). By decoupling the solutions for $\phi(x)$ and $\chi(x)$ we obtain:

$$(\alpha_0^2 \frac{\partial^2}{\partial x^2} + i b_0^2 x^2) \phi(x) = (E^2 - i \alpha_0 b_0) \phi(x),$$
$$(\alpha_0^2 \frac{\partial^2}{\partial x^2} + i b_0^2 x^2) \chi(x) = (E^2 - i \alpha_0 b_0) \chi(x).$$

Each equation above corresponds to quantum harmonic oscillator with complex energy spectrum. The solution of Eq. (13) gives complex quantized eigenenergy and eigenstates as:

$$E_n = \omega (1 + i) \sqrt{n},$$
$$\phi_n(x) = H_n(\beta x) e^{-|\beta|^2 x^2/2},$$

where $n$ is real integer. (normalization is set to 1 for simplicity). $\omega = \sqrt{\alpha_0 b_0}$, and $\beta = \sqrt{-\frac{\alpha_0}{\alpha_0}}$. $H_n$ are the Hermite polynomials with real (imaginary) argument for $\alpha_0$ and $b_0$ with opposite (same) sign (i.e. when $\beta$ is real (imaginary)). In the former case, we have fully localized eigenstates $\phi_n$ at the domain walls.

**Supersymmetric connection.** Its evident that $\chi_n(x)$ states are same as $\phi_n(x)$ with shifted eigenvalues:

$$E_n = \omega (1 + i) \sqrt{n + 1}. \tag{17}$$

In other words, the same $E_n$ eigenstate of both oscillators correspond to $n + 1$ and $n$ eigenstates of a harmonic oscillator for $\phi$ and $\chi$ excitations. This is qualitatively analogous to the supersymmetric like coupled oscillator solutions, but with complex energy spectrum.

**Conclusions.** Our work presented a number of important aspects of the $\mathcal{CPT}$ invariant quantum theory, including the dynamical nature of the $\mathcal{C}$ operator, and its unique consequences, $\mathcal{CPT}$ invariance gauge transformation, extension of the $\mathcal{PT}$ invariant quantum theory to spinful fermions, non-Abelian topological features, and an analogue of supersymmetric edge state solutions. We highlighted previously explored the dynamical nature of the $\mathcal{C}$ operator, and its crucial role on the conservation of probability in time-dependent systems, and the theory of $\mathcal{CPT}$ invariant gauge invariance and co-variance. The dynamical evolution of the $\mathcal{C}$ operator not only ensures probability conservations, but also contributes a new term to the Berry phase. We proposed a method of bypassing the hurdle of $T^2 = -1$ symmetry associated with
spin-1/2 fermions to obtain the \((PT)^2 = +1\) symmetry for NH Hamiltonians with real eigenvalues. We also find that the proposed spinfull Hamiltonian possess non-Abelian Berry gauge field and unique supersymmetric-like localized boundary states despite complex eigenvalues. Our work contributes to the development of complete \(CPT\)-invariant theory for dynamical systems, the evolution of geometric phase for spinfull systems, and sets up a pathway to achieve non-Abelian excitations without applied magnetic field or interactions.

**Supplementary Materials**

**Time evolution of \(PT\)-invariant systems**

Let us consider a linear time evolution of the eigenstates for a \(PT\)-symmetric system is

\[
i\hbar |\dot{\psi}(t)\rangle = Q(t)|\psi(t)\rangle,
\]

where \(Q(t)\) is a generic time-evolution operator. Dot denotes time-derivative. For the Hermitian case, \(Q(t) = H\). \(Q\) becomes different for a \(CPT\)-invariant system. The physical constraint to keep in mind is that the \(CPT\)-inner product of the system is a constant of motion, i.e., \(\partial_t \langle \psi_m | CPT | \psi_n \rangle = 0\) for all \(n\) and \(m\) eigenstates. This constraint dictates that

\[
\langle \psi_m | \dot{CPT} | \psi_n \rangle = -i \langle \psi_m | CPT | \psi_n \rangle - \langle \psi_m | CPT | \dot{\psi}_n \rangle.
\]

Using Eqs. (18) and (19), we obtain the equation of motion of the \(C\)-operator as

\[
i\hbar \dot{CPT} = [Q, CPT].
\]

(Eq. (20) can be equivalently written as \(i\hbar \dot{C} = [QC - CQ^{PT}]\) where \(QC^{PT} = (PT)Q(PT)^{-1}\) is understood to be \(PT\) conjugate.)

At this point, we can infer two properties of the \(Q\) operator. Firstly, Eq. (20) implies that unlike the Hamiltonian itself, \(Q\) is not, in general, \(CPT\)-invariant; otherwise \(C\) becomes a constant of motion. Secondly, in the above derivation we have used the symmetry property that \(\dot{Q} = Q\) (where \(T\) is the transpose), which is in accord with the symmetric Hamiltonian assumed here. (Otherwise, the derivation can also be proceeded with keeping the transpose operator throughout the derivation below.)

Since \(Q\) is a generic symmetric matrix, it can be expressed as a sum of a \(CPT\)-symmetric matrix (say, \(S\)), and a \(CPT\)-antisymmetric matrix (say, \(A\)): \(Q = S + A\), where \([S, CPT] = 0\) & \([A, CPT] = 0\). Since either \(S\) or \(A\) can be chosen arbitrarily, without losing generality, we set \(S = H\) for any \(CPT\)-symmetric Hamiltonian. Then \(A\) can be determined easily. Notice that for \(A\) to be antisymmetric with \(CPT\), it should follow either (i) \([A, P] = 0\) and \([A, C] = 0\), or (ii) \([A, P] = 0\) and \([A, C] = 0\). In both cases, we get from Eq. (20) that \(A = 2iC^{-1}\dot{C}\). Therefore, the final result of the time-evolution operator is

\[
Q = H + \frac{i\hbar}{2} C^{-1} \dot{C}.
\]

This is an important result which implies that that the time-evolution of the system is governed by both the Hamiltonian and the \(C\)-operator to make sure the probability of the state remains a constant of motion.

**Non-Abelian Berry matrix**

Let us assume the system adiabatically evolves in time such that the time-dependent Hamiltonian possess instantaneous eigenstates \(|\psi_n(t)\rangle\) satisfying

\[
H(t)|\psi_n(t)\rangle = E_n|\psi_n(t)\rangle.
\]

For generality, we assume each eigenstate is \(N\)-fold degenerate. (Since Berry phase does not depend on onsite energy, we set \(E_n = 0\) for simplicity. It can be shown that the result remains unchanged for \(E_n \neq 0\) as long as its real.) In the adiabatic limit, the total wavefunction \(|\phi_n\rangle\) can be expanded in terms of \(|\psi_n(t)\rangle\) as:

\[
|\phi_n(t)\rangle = \sum_m |\psi_m(t)\rangle \Gamma_{mn}(t).
\]

Substituting \(|\phi_n(t)\rangle\) in Eq. (18) with the time-evolution operator \(Q\) given in Eq. (21) we obtain

\[
\sum_m \left[ |\psi_m\rangle \Gamma_{mn} + |\psi_m\rangle \dot{\Gamma}_{mn} \right] = \frac{i}{2} e^{-i \frac{\dot{C}}{\hbar} \sum_m |\psi_m\rangle \Gamma_{mn}},
\]

where we have substituted \(H|\psi_n\rangle = 0\). Multiplying \(|CPT\psi_i\rangle\) from left, and using the orthonormal condition for the \(CPT\) inner products, we obtain

\[
\dot{\Gamma}_{in} = -\sum_m \left[ \langle \psi_i | CPT | \dot{\psi}_m \rangle - \frac{1}{2} \langle \psi_i | \dot{CPT} | \psi_m \rangle \right] \Gamma_{mn},
\]

where the non-Abelian Berry gauge field is defined as

\[
A_{lm} = i \left[ \langle \psi_l | CPT | \psi_m \rangle - \frac{1}{2} \langle \psi_l | \dot{CPT} | \psi_m \rangle \right].
\]

In the case when there is no explicit time-dependence, we write Berry gauge field as vector for each elements as

\[
A_{\mu,lm} = i \left[ \langle \psi_l | CPT | \partial_\mu \psi_m \rangle - \frac{1}{2} \langle \psi_l | (\partial_\mu C)PT | \psi_m \rangle \right],
\]

where \(\mu\) denotes spatial coordinates. Eq. (25) can be written in a matrix multiplication format as

\[
\dot{\Gamma} = i A \Gamma,
\]

where \(\Gamma\) and \(A\) are matrices of dimension \(N \times N\). Integration of Eq. (28) yields the Berry rotation matrix to be

\[
\Gamma = P e^{i \int A_{\mu} dx^\mu} = e^{i \gamma},
\]
where $P$ represents path-ordered product. $\gamma$ gives the non-Abelian Berry phase matrix whose components are defined by

$$
\gamma_{mn} = \int A_{\mu, mn} dx^\mu.
$$

(30)

Clearly, $m = n$ gives the Abelian component.

$U(N)$ gauge transformation and CPT co-variant derivative

Let $|\psi'_n\rangle$ be a different choice of the eigenstate which is related to the previous one by a $U(N)$ gauge transformation:

$$
|\psi'_n\rangle = \sum_m |\psi_m\rangle U_{mn}.
$$

(31)

The corresponding CPT conjugate of $|\psi'_n\rangle$ is defined as $\langle CPT \psi'_n(t) | = \sum_m (U^\dagger)^{CPT}_{nm} \langle CPT \psi_m(t) |$. (Although the transpose operator on $U$ can be taken into account simply by shuffling the indices $mn$ to $nm$, however, we explicitly retain the transpose symbol for easier derivation below. In most cases $U$ is a symmetric matrix, however, we can proceed without such an assumption for generality.) Given that the inner product must be invariant, i.e., $\langle \psi'_n | CPT | \psi'_m \rangle = \langle \psi_n | CPT | \psi_m \rangle$ under a $U(N)$ gauge transformation, we find that the $U(N)$ operator must follow

$$
(U^\dagger)^{CPT} U = I,
$$

(32)

where $T$ is again the usual transpose operator, and $I$ is the $N \times N$ identity matrix. This is equivalent to the unitary condition for the Hermitian case. From Eq. (27) we then obtain

$$
A'_{\mu, lm} = i \left[ \langle \psi'_l | CPT | \partial_{\mu} \psi'_m \rangle - \frac{1}{2} \langle \psi'_l | (\partial_{\mu} C) CPT | \psi'_m \rangle \right],
$$

$$
= i \sum_{l', m'} (U^\dagger)^{CPT}_{l'm'} \left[ \langle \psi_{l'} | CPT | \partial_{\mu} \psi_{m'} \rangle \right. \\
- \frac{1}{2} \langle \psi_{l'} | (\partial_{\mu} C) CPT | \psi_{m'} \rangle \left. \right] + \partial_{\mu} U_{l'm'} \langle \psi_{l'} | CPT | \psi_{m'} \rangle,
$$

$$
= \sum_{l', m'} (U^\dagger)^{CPT}_{l'm'} A_{\mu, l'm'} + i \partial_{l'} U_{l'm'} \partial_{\mu} U_{l'm'}. \quad (33)
$$

Eigenspectrum algebra of the Hamiltonian

The full Hamiltonian (Eq. (35)) is

$$
H_k = \begin{pmatrix}
\epsilon_k & i\alpha_k & b_{k^+} & 0 \\
-\alpha_k & \epsilon_k & 0 & b_{k^-} \\
b_{k^+} & 0 & \epsilon_k & -i\alpha_k \\
b_{k^-} & 0 & b_{k^+} & \epsilon_k
\end{pmatrix}.
$$

(35)

The eigenvectors in terms of the dispersion spectrum are:

$$
\psi_{1,3} = \frac{i}{\sqrt{2(d_k^2 - \alpha_k^2)}} \begin{pmatrix} \alpha \\
\pm \alpha d_k \\
\pm \alpha b_k \\
\pm \alpha b_k
\end{pmatrix},
$$

$$
\psi_{2,4} = \frac{1}{\sqrt{2(d_k^2 - \alpha_k^2)}} \begin{pmatrix} \alpha \\
\pm \alpha d_k \\
\pm \alpha b_k \\
\pm \alpha b_k
\end{pmatrix}. \quad (36)
$$

(k dependence is implicit above). Here we denote $b_{k^\pm} = (b_{k^+} \pm b_{k^-})/2$, and $b_{k||} = \sqrt{b_{k^+}^2 - \alpha_k^2}$, and $d_{k\pm} = b_{k\pm} \pm b_{k||}$. We next define a polar coordinate with complex angle as $b_{k^+} = b_{k||} \cosh \theta_k$, and $\alpha_k = b_{k||} \sinh \theta_k$. $\theta_k = \text{tanh} \left( \frac{\alpha_k}{b_{k^+}} \right)$. We notice an interesting feature of the angle $\theta_k$ here. The $PT$-symmetric region is defined by $\alpha_k/d_{k\pm} \leq 1$ rendering $\theta_k \to \infty$ at the $PT$-symmetric boundary. $\theta_k = \pi$ at $\alpha_k/d_{k^\pm} = \text{tanh}(\pi) = 0.9962720$ (a transcendental number), slightly below the $PT$ symmetric boundary.

In this polar coordinate of $(b_{k||}, \theta_k)$, we have $d_{k^+} = 2b_{k||} \cosh^2 \theta_k/2$, and $d_{k^-} = 2b_{k||} \sinh^2 \theta_k/2$. This gives $\sqrt{d_{k^+}^2 - \alpha_k^2} = 2b_{k||} \cosh \theta_k/2$, and $\sqrt{d_{k^-}^2 - \alpha_k^2} = 2b_{k||} \sinh \theta_k/2$. Substituting these identities in Eq. (36) we obtain the final expressions for the eigenstates in terms of the the angle $\theta_k$ only as:

$$
\psi_{1,3} = \frac{1}{\sqrt{2}} \begin{pmatrix} \sinh \left( \frac{\theta_k}{2} \right) \\
\pm \sin \left( \frac{\theta_k}{2} \right) \\
\pm \sinh \left( \frac{\theta_k}{2} \right) \\
\pm \sin \left( \frac{\theta_k}{2} \right)
\end{pmatrix}, \quad \psi_{2,4} = \frac{1}{\sqrt{2}} \begin{pmatrix} -i \cosh \left( \frac{\theta_k}{2} \right) \\
\pm \sin \left( \frac{\theta_k}{2} \right) \\
\pm \sinh \left( \frac{\theta_k}{2} \right) \\
\mp \sin \left( \frac{\theta_k}{2} \right)
\end{pmatrix}. \quad (37)
$$

For the operator $PT = (\gamma_0 \otimes \gamma_2)K$ where $K$ is the complex conjugation operator, we find $\langle PT \psi_n | = \langle \psi_n |$ for all all eigenstates $n$. The $PT$ inner products are $\langle PT \psi_m | PT \psi_n | = \langle \psi_m | PT \psi_n | = (-1)^m \delta_{mn}$. The $\mathcal{C}$ operator is defined accordingly as $\mathcal{C} = \sum_n \langle \psi_n | PT \psi_n | = (\gamma_0 \otimes \gamma_2) \cosh \theta_k + i \gamma_0 \gamma_2 \sinh \theta_k$. With this $\mathcal{C}$ operator we obtain the $CPT$-invariant quantum theory: $\langle \psi_m | CPT | \psi_n \rangle = \delta_{mn}$, and $\sum_n \langle \psi_n | CPT | \psi_n \rangle = I$.

It is interesting to identify a crucial correspondence between the $\psi_{1,3}$ and $\psi_{2,4}$ eigenstates: $\partial_k \psi_{1,3} = i \frac{\partial \theta_k}{2} \psi_{2,4}$, and $\partial_k \psi_{2,4} = i \frac{\partial \theta_k}{2} - \psi_{1,3}$. This correspondence guarantees the existence of non-Abelian Berry gauge field $A^T_{1,2} = A^T_{2,1} = \partial_k \theta_k$. The Berry connection is a real, symmetric matrix in the $PT$ symmetric region.
Edge state calculations

The bulk-boundary correspondence for the $\mathcal{PT}$-symmetric NH topological insulators is not as concrete as in the Hermitian case, and relies on systems under consideration as well as the symmetry invariance. This is quite evident because of the fact that the real eigenvalues, and conserved eigenstates in the bulk are protected by the $\mathcal{PT}$-symmetry (or rather the $\mathcal{CPT}$ symmetry), whereas such a symmetry may be inevitably lost at the boundary even if the system resides in the same parameter regime. Such a case also occurs in the present Hamiltonian. For the discussion of the boundary state, a suitable choice of basis is obtained to be as follows.

$$
\phi_{\pm k} = \frac{1}{2} \left( \psi_{R, k}^\dagger + i \psi_{L, k}^\dagger \right) \pm \frac{1}{2} \left( \psi_{R, k}^\dagger - i \psi_{L, k}^\dagger \right),
$$

$$
\chi_{\pm k} = \frac{1}{2} \left( i \psi_{R, k}^\dagger + \psi_{L, k}^\dagger \right) \pm \frac{1}{2} \left( i \psi_{R, k}^\dagger - \psi_{L, k}^\dagger \right). \quad (38)
$$

With a suitable choice of the spinor from the fermions as $\psi_{R, k}, \chi_{\pm k}$, and $\phi_{\pm k}$ are real constant parameters. This yields the coupled equation of motion as

$$
\begin{pmatrix}
0 & i b_+ + i \alpha_k & 0 & 0 \\
-ib_+ + i \alpha_k & 0 & 0 & 0 \\
0 & 0 & -ib_+ + i \alpha_k & 0 \\
0 & 0 & 0 & -ib_+ + i \alpha_k
\end{pmatrix} \begin{pmatrix}
\phi_k^R \\
\phi_k^L \\
\chi_k^R \\
\chi_k^L
\end{pmatrix} = E_k \begin{pmatrix}
\phi_k \\
\chi_k
\end{pmatrix} \quad (41)
$$

We substitute $\alpha^2 = -1/2m$, and $b_0 = k/2$, where $m$ and $k$ are to be thought of as mass and spring constant (with suitable dimension adjustment), respectively. We also substitute $E^2 + i \alpha \phi_0b_0 = \lambda^2$. Then the connection to the Harmonic oscillator becomes vivid. Following the same quantization condition of a quantum Harmonic oscillator we have $\lambda^2 = (n + \frac{1}{2}) \sqrt{k/\alpha}$, where $n$ is real integer. This gives the solutions of Eqs. (44) as complex quantized energy

$$
E_n = \omega(1 + i)\sqrt{n},
$$

$$
\phi_n(x) = AH_n(\beta x) e^{-|\beta| x^2/2}. \quad (46)
$$

$$
\omega = \sqrt{\alpha_0 b_0}, \quad \beta = \sqrt{-\frac{b_0}{\alpha_0}}. \quad A \text{ is the normalization constant.}
$$

$$
\text{For } \alpha_0 \text{ and } b_0 \text{ with opposite sign, we have perfectly localized solutions for both } \phi_n \text{ and } \chi_n \text{ states at the domain walls.}
$$

$$
\text{Its evident that } \chi_n(x) \text{ states are same as } \phi_n(x) \text{ with corresponding eigenvalues as}
$$

$$
E_n = \omega(1 + i)\sqrt{n + 1}. \quad (48)
$$

In other words, the $E_n$ eigenstates of both oscillators correspond to $n$ and $n + 1$ states of a harmonic oscillator for $\phi$ and $\chi$ excitations. This is the supersymmetric like coupled oscillators solutions, but with complex energy spectrum.

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