Topology of three-dimensional Dirac semimetals and generalized quantum spin Hall systems without gapless edge modes

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Introduction: The stable, three-dimensional, Dirac semimetals (DSM) arising from accidental linear touching between two Kramers-degenerate bands at isolated points in the Brillouin zone (BZ) are experimentally relevant examples of gapless topological states [11–19]. The Dirac points of such systems, occurring along an n-fold axis of rotation are protected by the combined PT and the n-fold, discrete, rotational (Cn) symmetries, with n = 3, 4, 6 [11, 12], where P and T represent space-inversion/parity (P) and time-reversal (T) symmetries, respectively. Several materials like Na3Bi [11–20], Cd3As2 [21, 22], PdTe2 [23], β’-PtO2 [16, 19], VAl3 [13, 14], β-CuI [13], K MGBi [12, 19], PtBi2 [31], and the magneto-electric (ME) compound FeSn [9, 32] can host such Dirac points. Despite intensive theoretical research on stable DSMs for almost ten years [11, 16, 18, 19], their bulk topological invariants are still unknown.

The simplest version of DSMs can be obtained by stacking of Bernevig-Hughes-Zhang (BHZ) model (34) of quantum spin Hall (QSH) effect along the direction of nodal separation or the Cn-axis. Since the BHZ model is a first order topological insulator (FOTI), supporting helical edge modes, the resulting DSM exhibits loci of zero-energy surface states, also known as the helical Fermi arcs. The total number of zero-modes is equal to the total QSH conductivity of DSMs, determined by ΔkF/π, where ΔkF is the distance between the bulk Dirac nodes. The spectroscopic and transport data of many stable DSMs are usually interpreted based on the existence of helical Fermi arcs [20–32].

However, recent theoretical works have showed that the generic, n-fold planes of DSMs are not described by the BHZ model possessing U(1) spin-conservation law, or closely related Z2 FOTIs [34]. Away from the mirror planes, various crystalline-symmetry-preserving perturbations can gap out the helical edge modes. Using K-theory analysis, the generic planes were found to be topologically trivial [4]. Subsequently, various groups [17, 19] have identified these planes as higher-order, topological insulators (HOTI) [35]. The distinction between FOTI and HOTI is established by computing the nested Wilson loops of SU(2) Berry connections for the occupied valence bands, under periodic boundary conditions. However, this difference only affects the physical properties under open boundary conditions, such as the presence of corner-states under Cn-symmetric open boundary conditions.

Are there any common topological properties shared by two-dimensional FOTI and HOTI under periodic boundary conditions? What happens to the QSH effect of the BHZ model, when the helical edge modes get gapped out by crystal-symmetry-preserving perturbations? We answer these two fundamental questions and identify the stable bulk topology of DSMs by performing second homotopy classification of non-Abelian Berry connections.

Challenge toward topological classification: The minimal model of a pair of two-fold, Kramers-degenerate bands of PT symmetric systems is described by the Hamiltonian H = ∑k Ψ†(k)H(k)Ψ(k), where Ψ(k) is a four-component spinor, and the Bloch Hamiltonian operator can be written as H(k) = N0(k)1 + ∑j=1 Nj(k)Γj [36, 39]. The magnitude of O(5) vector field N(k) controls the spectral gap between conduction and valence bands, N0(k) describes particle-hole anisotropy, and Γj are five, mutually anti-commuting, 4 × 4 matrices, such that {Γi, Γj} = 2δij. The topology of Bloch wave functions are determined by the unit, O(5) vector field N(k) = N(k)/|N(k)|, representing the coset
space \( SO(5)/SO(4) = S^4 \), where \( S^4 \) is the unit four-sphere. The diagonalizing matrix belongs to this coset space and the gauge group for intra-band Berry’s connection is given by \( Spin(4) = SU(2) \times SU(2) \).

The vanishing of \( N(k) \) restores \( SO(5) \)-symmetry at the Dirac points, which serve as singularities of \( N(k) \). Whether the Dirac points are monopoles of Berry connection, leading to the quantized Berry flux for generic \( n \)-fold planes, can only be unambiguously determined by performing second homotopy classification of the gauge group. Since \( \pi_2(S^4) \) and \( \pi_2(SU(2)) \equiv \pi_2(S^3) \) are trivial, the homotopy analysis involves conceptual subtleties. We will show that the form of \( C_n \) operator can be exploited to identify a pair of global spin-quantization axes and reduce the redundancy of band eigenfunctions from \( Spin(4) \) to \( U(1) \times U(1) \), which allows second homotopy classification.

**Model:** We substantiate these claims by considering a model of \( C_4 \)-symmetric, magneto-electric DSMs, arising from the hybridization between \( s \) and \( p \) orbitals, which does not support any gapless surface states. We will employ the following representation of gamma matrices 
\[
\Gamma_{1,2,3} = \tau_1 \otimes \sigma_j, \quad \Gamma_4 = \tau_2 \otimes \sigma_0, \quad \Gamma_5 = \tau_3 \otimes \sigma_0.
\]
The ten commutators \( \Gamma_{jm} = [\Gamma_j, \Gamma_m]/(2i) \), with \( j = 1, \ldots, 5 \) and \( l = 1, \ldots, 5 \) serve as the generators of \( SO(5) \) and its double cover group \( Spin(5) \). The \( 2 \times 2 \) identity matrix \( \tau_0 \) and the Pauli matrices \( \tau_j \) (\( \sigma_j \)’s), with \( j = 1, 2, 3 \) operate on orbital/parity (spin) index. The relevant \( O(5) \) vector is given by

\[
N(k) = \begin{bmatrix} t_p \sin k_x, t_p \sin k_y, t_d, \cos k_x - \cos k_y, & \cos \theta(k) g^+(-iuv \nabla u) g_+ - i g^+_u \nabla g_+, \\
& i \sin \theta(k) u(k) g_-(-iuv \nabla u) g_-, \cos \theta(k) g_-(-iuv \nabla u) g_- + ig^+_u \nabla g_+ \end{bmatrix}
\]

where \( t_s, t_p, t_{d1}, t_{d2} \) are four independent hopping parameters, and the dimensionless parameter \( \Delta \) controls topological phase transitions. The phase diagram is shown in Fig. 1(a). The DSMs (1 < \( |\Delta| < 3 \)) interpolate between trivial insulators (\( |\Delta| > 3 \)) and topological insulators (\( |\Delta| < 1 \)). We will focus on the parameter regime 1 < \( |\Delta| < 3 \), with the Dirac points located at \( k_D = (0, 0, \pm k_D) \), with \( \cos(k_D) = (\Delta - 2) \). Away from the high-symmetry locations \( k_D = 0, \pi \), the generic 4-fold planes of DSMs [3], preserving both \( P \) and \( T \) symmetries display identical form of \( N(k) \).

**Gauge-invariant Berry curvature:** The \( P \mathcal{T} \) symmetry is implemented by \( \Gamma_{24} \hat{H}(k) \Gamma_{24} = \hat{H}(k) \), and the diagonalizing matrix \( U(k) \) must satisfy the constraints \( U^\dagger(k) \hat{H}(k) U(k) = |N(k)| \Gamma_3 \), and \( U^\dagger(k) \Gamma_{24} U(k)^* = \Gamma_{24} \). Hence, \( U(k) \in Spin(5)/Spin(4) \) has the general form [33, 39],

\[
U(k) = \begin{bmatrix} \cos \theta(k)/2 g^+(-iuv \nabla u) g_+ & i \sin \theta(k)/2 u(k) g_-(-iuv \nabla u) g_- \\
i \sin \theta(k)/2 u(k) g_+(-iuv \nabla u) g_+ & \cos \theta(k)/2 g_-(-iuv \nabla u) g_- \end{bmatrix}
\]

where the first (last) two columns correspond to the eigenfunctions of conduction (valence) bands. We have parametrized \( S^4 \) with a polar angle \( \theta(k) \) and a four-component unit vector \( \hat{n}_\mu \), with \( \mu = 1, 2, 3, 4 \), such that \( \cos[\theta(k)] = \frac{N_3(k)}{N(k)}, \) and \( \hat{n}_\mu = \frac{N_\mu(k)}{N(k)|\sin[\theta(k)]|} \). The \( SU(2) \) matrix \( u(k) = i \bar{n}_4(k) \sigma_0 + i \bar{n}_3(k) \sigma_2 \) describes the hybridization matrix elements between two orbitals, while two \( SU(2) \) matrices \( g_\pm(k) \) describe gauge freedom in selecting the eigenfunctions for conduction and valence bands, respectively. From \( U(k) \) one finds the following intra-band \( SU(2) \) connections

\[
A_+(k) = \frac{\sin^2 \theta}{2} g_+^{\dagger}(-iuv \nabla u) g_+ - ig^+_u \nabla g_+,
\]

\[
A_-(k) = \frac{\sin^2 \theta}{2} g_-^{\dagger}(-iuv \nabla u) g_- - ig^+_u \nabla g_-,
\]

for the conduction and valence bands, respectively. For notational compactness, we have suppressed the explicit \( k \)-dependence of \( \theta, u, \) and \( g_\pm \).

The \( C_4 \) symmetry requires \( C_4 \hat{H}(k) C_4^\dagger = \hat{H}(k') \), which implements the constraint \( U^\dagger(k') C_4 U(k') = \Gamma_5 \), with the rotated vector wave \( k' = (-k_x, k_x, k_2) \). For the orbital basis, \( C_4 = e^{i\theta_0 \sigma_3} \otimes e^{i\theta_4 \sigma_3} \), with \( \theta_0 = \pi/2(2p + 1) \), \( \theta_4 = \pi/2(2q + 1) \), and \( p = 2 \text{ mod 4} \) and \( q = 0 \text{ mod 4} \), and the hybridization matrix \( u \) transforms as \( u(k') = e^{i\theta_0 \sigma_3} u(k) e^{-i\theta_4 \sigma_3} \). In the band basis, the transformed rotation operator \( C_4 \) becomes

\[
C_4^\dagger(k') \equiv U^\dagger(k') C_4 U(k) \]

and the gauge choices \( g_\pm(k) = \sigma_0 \) and \( g_\pm(k) = e^{i\alpha_\pm(k)} \sigma_3 \), keep the spin quantization axes unaffected.

Any general choice of gauge specify a pair of local spin quantization axes \( \hat{m}_\pm(k) \), according to \( g_\pm(k) \sigma_3 g_\pm(k) = \hat{m}_\pm(k) \cdot \sigma \). Once \( g_\pm(k) \) are identified, \( U(k) \) only exhibits residual \( U(1) \times U(1) \) gauge freedom, corresponding to the spin rotations about \( \hat{m}_\pm(k) \), i.e., \( g_\pm(k) \to g_\pm(k) \exp[\pm ig_\pm(k) \hat{m}_\pm(k) \cdot \sigma] \). Consequently, the gauge group of intra-band Berry connection is given by \( Spin(4)/[U(1) \times U(1)] \), with the second homotopy class

\[
\pi_2 \left( \frac{Spin(4)}{U(1) \times U(1)} \right) = \pi_1(U(1) \times U(1)) = \mathbb{Z} \times \mathbb{Z}. \tag{5}
\]

Hence, the topology of \( n \)-fold planes and the Dirac points are governed by a pair of integer invariants, and the Dirac points can be identified as non-Abelian monopoles.

The Abelian projected Berry connections can be obtained as \( A_+(k) = \frac{i}{2} Tr[\bar{A}_+(k) \hat{m}_\pm(k) \cdot \sigma] = \frac{i}{2} Tr[C_4^\dagger(g_\pm(k) \sigma_3 \sigma_\pm g_\pm(k))] \), leading to

\[
\bar{A}_+(k) = \frac{i}{2} \sin^2 \theta Tr[-iu \nabla u \sigma_3] + i \frac{1}{2} Tr[g^+_u \nabla g_+ \sigma_3],
\]

\[
\bar{A}_-(k) = \frac{i}{2} \sin^2 \theta Tr[-iu \nabla u \sigma_3] + i \frac{1}{2} Tr[g^+_u \nabla g_- \sigma_3]. \tag{6}
\]
Consequently, the gauge-invariant, quantized Berry flux can be determined from the Abelian field strength tensors (or Berry curvatures) $F_{ij,\pm}(k) = \partial_i A_{j,\pm}(k) - \partial_j A_{i,\pm}(k)$. For all smooth gauge transformations, such that the spin quantization axes are topologically trivial, meaning the gauge-fixing operators $\hat{\mathbf{m}}_{\pm}(k) \cdot \sigma$ do not correspond to fictitious two-band models of Chern insulators, $i/2Tr[g_{ij}\nabla g_{\pm} \sigma_3]$ terms cannot contribute to the quantized flux of $\bar{F}_{ij,\pm}(k)$ or the relative Chern numbers for 4-fold planes, defined as

$$\mathcal{C}_{R,\pm}(k_z) = \frac{1}{2\pi} \int_{T^2} dk_x dk_y \bar{F}_{xy,\pm}(k).$$

Quantized Berry flux: Next, we perform explicit analytical calculations of Berry flux with the global gauge choice $g_{\pm}(k) = \sigma_0$, corresponding to the spin quantization axes $\hat{\mathbf{m}}_{\pm}(k) = (0, 0, 1)$. It is convenient to define symmetric and anti-symmetric combinations of Berry curvatures as $\bar{F}^{ij}_{12} = (\bar{F}_{ij, +} + \bar{F}_{ij, -})/2$, and $\bar{F}^{34}_{ij} = (\bar{F}_{ij, +} - \bar{F}_{ij, -})/2$. These curvatures will be associated with the diagonal, Cartan generators of $SO(5)$ group, namely $\Gamma_{12} = \tau_0 \otimes \sigma_3$ and $\Gamma_{34} = \tau_3 \otimes \sigma_3$, and can be elegantly written as $\bar{F}^{ab}_{ij} = \sin(\theta_{ab})[\partial_i \theta_{ab} \partial_j \phi_{ab} - \partial_i \phi_{ab} \partial_j \theta_{ab}]$, where we have introduced two sets of spherical polar angles $(\theta_{12}(k), \phi_{12}(k))$ and $(\theta_{34}(k), \phi_{34}(k))$, such that

$$\tan[\phi_{ab}(k)] = \frac{N_{\phi}(k)}{N_{\theta}(k)},$$

$$\cos[\theta_{ab}(k)] = 1 - \frac{[N_{\phi}^2(k) + N_{\theta}^2(k)]}{[N(k)[N(k) + N_{5}(k)]]}. \tag{9}$$

The quantized flux of $\bar{F}^{12}_{ij}$ and $\bar{F}^{34}_{ij}$ can only exist if BZ
two-torus can wrap around unit two spheres, defined by
\[ \mathbf{n}_{ab} = (\sin \theta_{ab} \cos \phi_{ab}, \sin \theta_{ab} \sin \phi_{ab}, \cos \theta_{ab}) \].

Notice that \( \Phi_{12}^{z}(k_z) = 2\pi \mathcal{C}_{R,12}(k_z) \) and \( \Phi_{34}^{z}(k_z) = 2\pi \mathcal{C}_{R,34}(k_z) \) describe the flux of Abelian fields \( \mathcal{F}_{12} \) and \( \mathcal{F}_{34} \), respectively.

For all topologically non-trivial 4-fold planes of \( \mathcal{C}_4 \)-symmetric DSMs described by Eq. (1), only \( \theta_{12} \) interpolates between 0 and \( \pi \), leading to the skyrmion configuration for the unit vector \( \mathbf{n}_{12} \), as shown in Fig. 1(b). In contrast to this, \( \theta_{34} \) does not interpolate between 0 and \( \pi \), and the corresponding unit vector \( \mathbf{n}_{34} \) is topologically trivial, as shown in Fig. 1(e). The quantization of the relative Chern numbers, and their discontinuities at the Dirac points are shown in Fig. 1(d). The monopole numbers for the Dirac points at \( k = (0, 0, \pm k_{D,j}) \) are determined by \( \mathcal{N}_{12}(\pm k_{D,j}) = \lim_{\epsilon \to 0} \left[ \mathcal{C}_{R,12}(k_z = \pm k_{D,j} + \epsilon) - \mathcal{C}_{R,12}(k_z = \pm k_{D,j} - \epsilon) \right] = \pm 1 \), and \( \mathcal{N}_{34}(\pm k_{D,j}) = 0 \).

In Fig. 1(e) we illustrate the structure of Abelian projected magnetic fields \( B_{12}^{\phi}(k) = \frac{1}{4} \epsilon_{ijl} F_{ij}^{12}(k) \), which support dipole configuration. Using the \( k_z \)-dependent relative Chern numbers, we can also define the average relative Chern numbers per \( xy \) plane \( \left( \mathcal{C}_{R,ab}(\Delta) = \frac{1}{2\pi} \int_{\Delta} d^2 k_z \mathcal{C}_{R,ab}(k_z) \right) \), which is shown in Fig. 1(f). We note that the stacked BHZ model with \( t_{d,1} = t_{d,2} = 0 \), the stacked HOTI with \( t_{d,2} = 0 \) and the stacked HOTI with \( t_{d,1} = 0 \) support identical quantized flux of \( F_{ij}^{12}(k) \).

Hence, the relative Chern number acts as a topological order parameter for various phases, controlling the strength of generalized QSH effect, which can be seen in the following manner.

**Generalized QSH effect:** Refs. 40–43 have identified spin-charge separation as the non-perturbative signature of QSH, which can survive as a genuine topological response even in the absence of \( U(1) \) spin conservation law. For the BHZ model \( (t_{d,1/2} = 0) \) and closely related \( Z_2 \) FOTI, supporting gapless edge modes, it was shown that an electromagnetic \( \pi \) flux tube binds two-fold degenerate, zero-energy, mid-gap states. When both states are occupied (empty), the Kramers-singlet, ground state carries charge \( +e \) (\( -e \)). In contrast to this, the half-filling of zero-modes corresponds to Kramers-doublet with charge \( e = 0 \).

To demonstrate spin-charge separation for \( \mathcal{C}_4 \)-symmetric HOTI, we have computed the local density of states in the presence of an electromagnetic flux tube, oriented along the \( z \)-axis, for a system size \( 21 \times 21 \), under periodic boundary condition. The local density of states at the location of flux tube is shown in Fig. 2(a) as a function of energy and the strength of flux \( \phi \). The calculations were performed with hopping parameters \( t_x = t_p = t_{d,1} = t_{d,2}, k_z = \pi/2 \), and \( \Delta = 1.5 \). The low-energy states for \( \phi = \phi_0/2 \) i.e., \( \pi \)-flux are shown in Fig. 2(b) providing clear evidence for the existence of two-fold degenerate, mid gap states at zero-energy. All topologically non-trivial planes of DSMs can support such mid-gap states (which may or may not be at zero energy), and their total number corresponds to \( \Delta k_{B}/\pi \). Therefore, the relative Chern number provides a unified theoretical framework for describing generalized QSH effect of Kramers-degenerate FOTI and HOTI, irrespective of the presence or absence of gapless edge-modes and corner-localized states.

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