The three-dimensional, stable Dirac semimetals (DSM) are experimentally relevant examples of gapless topological states, which arise from linear touchings between two Kramers-degenerate bands at isolated points of Brillouin zone (BZ). Despite intensive theoretical research on stable DSMs for almost ten years,[14,22] their bulk topological invariants are still unknown. The wealth of spectroscopic and transport data on stable DSMs have been widely interpreted based on the approximate theory of decoupled Weyl semimetals (WSM).[23–34] While this approach is useful for addressing thermodynamic scaling laws at low temperatures, it is inadequate for describing topological properties of DSMs.

The Weyl points, arising from linear touchings between two non-degenerate bands are hedgehog defects of a three-component or O(3) vector field and Abelian Berry’s connections. They cause local restoration of SO(3)-symmetry at isolated points of momentum space. In contrast to this, the Dirac points are point defects of a five-component or O(5) vector field and non-Abelian, SO(5)-symmetry breaking and its restoration in reciprocal space are also essential for understanding the topological properties of DSMs.

The primary goals of our current work are to (i) develop gauge-invariant descriptions of bulk topological properties of stable DSMs, and (ii) outline a general recipe for computing bulk invariants, without relying on surface-states. We show the surface-states of DSMs generally possess intertwined signatures of Dirac points and additional, crystalline-symmetry-enforced defects of O(5) vector, such as mirror planes. Therefore, we use exact solutions of surface-states to outline their fermiology and spin-orbital textures, which are directly measured by angle-resolved-photoemission spectroscopy. The spin-
orbital textures are shown to carry detailed information about the underlying order. The research on three-dimensional DSMs began by considering the universality class of quantum phase transitions between two topologically distinct, insulating states. \[^{10,21}\] In Bi\(_{1-x}\)Sb\(_x\) \[^{10,21}\] and BiTeI(S\(_1-x\)Se\(_x\)) \[^{12,14}\] (Bi\(_{1-x}\)In\(_x\))\(_2\)Se\(_3\) \[^{15,19}\]\(^{15,19}\), the transitions between strong topological and trivial insulators are controlled by unstable DSMs, with an odd number of band-touchings at time-reversal-invariant momentum (TRIM) points. Moreover, the unstable DSMs, with an even number of Dirac points can describe transitions between topological-crystalline-insulators and trivial insulators, in a material like Pb\(_{1-x}\)Sn\(_x\)Te \[^{20,21}\].

The possibility of realizing stable DSMs, where the Dirac points occur at TRIM locations of BZ, along an axis of rotation, with \(n = 3, 4, 6\). These Dirac points are protected by the combined \(\mathcal{P}\mathcal{T}\) and the \(n\)-fold, discrete rotational (\(C_n\)) symmetries. Such DSMs have been experimentally realized in several materials. The Dirac materials like Na\(_3\)Bi \[^{31,32,26}\], Cd\(_3\)As\(_2\) \[^{17,12}\], PdTe\(_2\) \[^{23}\], \(\beta\)-PbO\(_2\) \[^{20,22}\], VA\(_3\) \[^{45}\], \(\beta\)-CuI \[^{17}\], KMg\(_2\)Bi\(_4\) \[^{12,22}\], and Pt\(_3\)Bi\(_2\) \[^{52}\] separately preserve \(\mathcal{P}\) and \(\mathcal{T}\) symmetries. By contrast, the magneto-electric (ME) Dirac material Fe\(_3\)S\(_4\) \[^{13,24}\] breaks \(\mathcal{P}\) and \(\mathcal{T}\), but preserves \(\mathcal{PT}\). In this work, we will focus on the topological classification of such DSMs, arising from accidental band-touchings.

**A. Challenges toward topological classification**

The real challenge toward topological classification of DSMs can be understood in the following manner. The minimal model of two Kramers-degenerate bands is described by the Hamiltonian \(H = \sum_k \Psi^\dagger(k) \hat{H}(k) \Psi(k)\), where \(\Psi(k)\) is a four-component spinor, and the Bloch Hamiltonian operator can be written as \(\hat{H}(k) = \sum_{j=1}^5 N_j(k) \Gamma_j\), \(^{13,33,53}\)])\(^{13,33,53}\]. The five-component (or \(O(5)\))-vector field \(\mathbf{N}(k)\) encodes details of band-structures and \(\Gamma_j\)'s are five, mutually anti-commuting \(4 \times 4\) matrices, such that \([\Gamma_i, \Gamma_j] = 2\delta_{ij}\). For concreteness, let us consider

\[
\mathbf{N}(k) = \begin{bmatrix}
    t_p \sin k_x & t_p \sin k_y & t_{d,1} \sin k_z & (\cos k_x - \cos k_y) \\
    t_{d,2} \sin k_x & t_{d,2} \sin k_y & t_s (\Delta - \sum_{j=1}^3 \cos k_j)
\end{bmatrix},
\]

which describes \(C_4\)-symmetric DSMs, arising from hybridizations between \(s\)- and \(p\)- orbitals. Here, \(t_p, t_p, t_{d,1}, t_{d,2}\) are four independent hopping parameters, and the dimensionless parameter \(\Delta\) controls topological phase transitions. When \(1 < \Delta < 3\), all five components of \(\mathbf{N}(k)\) vanish at the Dirac points, located at \(k = (0, 0, \pm k_d)\), with \(\cos k_d = (\Delta - 2)\).

Away from the Dirac points, the spectral gap \(2\left|\mathbf{N}(k)\right|\) between conduction and valence bands is governed by the amplitude of \(\mathbf{N}(k)\), while the properties of Bloch wave functions are determined by the unit vector field \(\mathbf{N}(k) = N_j(k)/\left|\mathbf{N}(k)\right|\). This corresponds to a pattern of symmetry breaking \(SO(5) \to SO(4)\), described by the coset space \(SO(5)/SO(4) = S^4\), where \(S^4\) is the unit, four-sphere. On the fermionic spinor \(\Psi(k)\), the action of special orthogonal groups \(SO(5)\) and \(SO(4)\) are realized in terms of their respective double cover groups \(Spin(5) = USp(4)\), and \(Spin(4) = SU(2) \times SU(2)\). The ten commutators \(\Gamma_{ij} = [\Gamma_i, \Gamma_j]/(2i)\), with \(i = 1, ..., 5\) and \(l = 1, ..., 5\), and \(j \neq l\) serve as the generators of \(SO(5)\) and \(Spin(5)\) groups. Since \(\hat{H}(k)\) can be diagonalized by unitary, \(Spin(5)\)-transformations, leaving local \(SU(2)\) redundancies of wave functions for both conduction and valence bands, the diagonalizing matrix is an element of \(SO(5)/SO(4) = Spin(5)/Spin(4) = S^4\), and the gauge group of intra-band Berry’s connections is given by \(Spin(4) = SU(2) \times SU(2)\). This coset space is also known as the quaternionic-projective-space \(HP^1\). \(^{53,56}\) The vanishing of amplitude \(\left|\mathbf{N}(k)\right|\) causes restoration of \(SO(5)\)-symmetry at the Dirac points, and they serve as singularities of \(O(5)\)-unit vector \(\mathbf{N}(k)\), and non-Abelian, \(SO(5)/SO(4)\)-Berry’s connections.

Can the Dirac points be identified as a pair of \(SO(5)\) monopole and anti-monopole? If they are monopoles, the resulting dipole configuration should support quantized, non-Abelian or chromo-magnetic, Berry’s flux through all \(xy\) planes, which are lying between two Dirac points \((|k_z| < k_d)\). By contrast, the \(xy\) planes, lying outside the Dirac points \((|k_z| > k_d)\), and all \(yz\) and \(xz\) planes would possess zero flux. This is a fundamental requirement of Gauss’s law. At a formal level, the topological quantization of flux through any closed surface, surrounding a singular point is determined by the second homotopy group \(\pi_2(G/H)\), where \(G/H\) is the coset space of gauge connections. The quantization of flux through generic \(xy\) planes (or classification of maps from \(T^2\) to \(G/H\)) is also determined by \(\pi_2(G/H)\). However, \(\pi_2(S^n)\) is trivial, for all \(n > 2\), and its naive application cannot determine the topological invariants of Dirac points or generic planes of DSMs.

Owing to these difficulties, the DSMs are often approximated by a pair of decoupled Weyl semimetals (WSMs) \[^{33,31,10}\] or the stacked, Bernevig-Hughes-Zhang (BHZ) model \[^{22}\]. This is motivated by the low energy approximation of massless Dirac fermions by a pair of Weyl fermions of opposite chirality. Such approximate theories
ignore two components of $\mathbf{N}(k)$, leading to

$$\mathbf{N}'(k) = [t_p \sin k_x, t_p \sin k_y, 0, 0, t_n(\Delta - \sum_{j=1}^{3} \cos k_j)] \tag{2}$$

and introduce a $U(1)$ chiral symmetry, with respect to $\Gamma_{12}$. Hence, the coset space is globally deformed from $S^2 \rightarrow SO(3)/SO(2) = SU(2)/U(1) = S^2$, which admits second homotopy classification according to $\pi_2(S^2) = \mathbb{Z}$, where $\mathbb{Z}$ is the group of integers. Notice the resulting gauge group of intra-band, Berry’s connection is Abelian. The integer winding number of three-component, unit vector $\mathbf{N}'(k)$ describes quantized, Abelian Berry’s flux ($\pm 2\pi$) for non-trivial $xy$ planes, lying between two Dirac points. This flux is associated with the generator $\Gamma_{12}$. Since the $\frac{1}{2} \text{Tr}[(1 \pm \Gamma_3)\Gamma_{12}] = 0$, the quantized flux defines a relative Chern number, which controls the non-dissipative, Hall transport of conserved quantity $\Psi^{\dagger} \Gamma_{34} \Psi$ (conserved $U(1)$ spin). Hence, the $xy$ planes of stacked BHZ model are quantum, spin Hall insulators and the Dirac points carry monopole charge $\pm 1$ with respect to $\Gamma_{12}$.

The non-trivial $xy$ planes of decoupled model support helical edge states, which display band crossings at $k_z = 0$ and $k_y = 0$. This leads to the loci of two-fold degenerate, zero-energy states, along the $\hat{z}$ axis, connecting the projections of bulk Dirac points on the (100) and (010) surface Brillouin zones (SBZs). These loci are known as the helical Fermi arcs. Various spectroscopic and transport measurements on Dirac materials have attempted to detect helical Fermi arcs, as the smoking gun evidence of bulk topology. However, the decoupled theories are insufficient for addressing global properties of Bloch wave functions. As soon as we consider the effects of various crystalline-symmetry-allowed perturbations ($t_{d,1} \neq 0$, and $t_{d,2} \neq 0$), the coset space reverts to $S^4$. Recent theoretical works have shown the helical Fermi arcs can be gapped out by the crystalline-symmetry-preserving perturbation $t_{d,1} \sin k_z$ ($\cos k_z - \cos k_{d}$) \text{[10,11,18,22以外]). Therefore, the spectroscopic and transport measurements on surface-states of DSMs should not be interpreted in terms of helical Fermi arcs.}

Some groups have avoided the drawbacks of low energy theories by focusing on the homotopy classification of $k_z = 0, \pi$ mirror planes. When allowed by the underlying point groups ($C_{4h}, D_{4h}, C_{6h},$ and $D_{6h}$ etc.), two components of $\mathbf{N}(k)$ vanish at these planes [$N_2(k)$ and $N_4(k)$ for the current example], causing restoration of $O(2)$ symmetry. Hence, they are crystalline-symmetry-enforced, planar topological defects of $\mathbf{N}(k)$ field, which can be classified by mirror Chern numbers.\text{[21,29]. For addressing the topology of Dirac points, we must perform classification of two-dimensional, insulators, described by the $O(5)$ vector, for $k_z \neq \{0, \pi\}$.

In Ref.\text{[7]} the change of $C_n$ eigenvalues of occupied valence bands, along the nodal direction (\hat{z} axis) has been used for defining the topological charge of Dirac points. This method relies on zeroth homotopy and no direct relationship with underlying Berry’s connections was established. Gorbar \textit{et al.} have considered the singular behaviors of gauge-covariant $SU(2)$ curvatures of conduction and valence bands, by employing continuum approximation of DSMs.\text{[22] But, the gauge-covariant curvatures cannot be used for defining topological invariants. Using $K$-theory analysis for $D_{4d}$ and $D_{6h}$-symmetric models of DSMs, Kargarian \textit{et al.} have showed the non-mirror planes are topologically trivial. Very recently, Refs.\text{[21,22] have proposed the $xy$ planes, with $|k_z| < k_d$, are examples of higher-order, topological insulators. In Ref.\text{[21] Szabo \textit{et al.} have discussed the possibility of hinge-localized, dispersive modes, without assigning any bulk topological invariant. In Ref.\text{[22] Wieder \textit{et al.} have performed topological classification of $SU(2)$ Berry’s connections of occupied valence bands, by calculating straight Wilson lines or Polyakov loops $W_x(k_y, k_z)$ and $W_y(k_x, k_z)$, along the principal axes $\hat{x}$ and $\hat{y}$. They have shown the gauge-invariant eigenvalues of $W_x(k_y, k_z)$ and $W_y(k_x, k_z)$ do not display 0 to 2$\pi$ windings, which are consistent with the absence of helical Fermi arcs. Consequently, they have addressed the topological properties of gauge-dependent generators of Wilson lines, by computing nested Wilson loops. While this is an interesting method for addressing topological obstructions, the straight Wilson lines are not the appropriate diagnostic tools of non-Abelian flux.}

\textbf{B. Summary of main results}

The insufficiencies of currently available theoretical methods have motivated us to perform \textit{second homotopy classification of DSMs}. Our main results are as follows.

1. First we provide a physically appealing description of quantized, non-Abelian flux, after performing Abelian gauge fixing with respect to the generators of $C_n$ symmetry. Such gauge fixing procedure modifies the gauge group of intra-band connections from $\text{Spin}(4)$ to $\text{Spin}(4)/U(1) \times U(1)$. This implies a sequence of symmetry breaking $\text{Spin}(5) \rightarrow \text{Spin}(4) \rightarrow U(1) \times U(1)$. Since $\pi_2(\text{Spin}(4)/U(1) \times U(1)) = \mathbb{Z} \times \mathbb{Z}$, the topology of Dirac points and all $xy$ planes can be classified by \textit{two integer winding numbers}.\text{[23] Based on this second homotopy classification, we identify the monopole charge of Dirac points, and the quantized flux through $xy$ planes. Various models of DSMs for $C_{4v}$- and $C_{6v}$-symmetric systems are then organized into distinct topological universality classes.}

2. For general readers, the broad idea behind such classification scheme can be described in the following manner. Depending on the underlying rotation eigenvalues of hybridizing orbitals, the linearized theory of DSMs can take one of the following two
3. Subsequently, we describe a computationally efficient tool of non-Abelian flux. We determine the non-Abelian, Berry’s phase by calculating planar Wilson loop (PWL) along a closed curve $C$, lying in the $xy$ plane, parametrized as $k(l)$. Here, $P$ denotes path ordering and $a_j(k(l))$’s correspond to intra-band, Berry’s connections. We mostly use $C_4$-symmetric loop whose center coincides with that of two-dimensional BZ. The PWL is sensitive to the existence of non-Abelian flux and serves as the appropriate generalization of Abelian Berry’s phase. For a topologically non-trivial plane, the gauge-invariant, spectra of $\log|W_C|/i$ show 0 to $2\pi$ windings, as the size of the loop is systematically increased to cover the entire two-dimensional BZ. The topologically trivial planes do not display such windings. Furthermore, we show the spectra of PWLs are independent of the chosen orientation on $S^4$ and remain invariant under $SO(5)$-gauge transformations. Since this method does not require any detailed knowledge of the underlying basis, it can be efficiently used for diagnosing bulk topology from ab initio band-structures of various Dirac materials. In contrast to the Abelian projections, this method can only detect the absolute magnitude of flux.

4. Our analysis shows the stability of monopole charge and quantized, Berry’s flux of $SO(3)$ models, when they are embedded in a larger $SO(5)$ group. But, the embedding dramatically modifies the windings of gauge-invariant spectra of Polyakov loops, along the principal axes of BZ. Thus, the gapless, surface-states spectra of decoupled WSMs or stacked BHZ model are not stable against the embedding.

5. Therefore, we perform exact analytical and numerical solutions of surface-states for different types of DSMs. *We show the generic $xy$ planes lying between two Dirac points only support gapped edge states, leading to the non-existence of helical Fermi arcs or the loci of zero-energy, surface-states.* Using the exact surface-states-Hamiltonians, we predict the fermiology and the in-plane, spin-orbital textures, which are directly measured by the spin-polarized angle-resolved-photoemission spectroscopy. The experimental relevance of gapped edge spectra of topologically non-trivial $xy$ planes are emphasized.

6. We also discuss the close relationship between the surface-states-Hamiltonians and the generators of Polyakov loops of Berry’s connections along principal axes of BZ. In spite of their resemblance, they are not topologically equivalent. The distinction arises, as the Polyakov loops are insensitive to the actual normalizability conditions of surface states.

Our paper is organized as follows. In Sec. [III] we describe different tight-binding models for $C_4$-symmetric DSMs and their global phase diagram. The structure of singular, $Spin(4)$-Berry’s connections are discussed in Sec. [IV]. In Sec. [V] we describe second homotopy classification of singular Berry’s connections with Abelian gauge fixing. Various models of $C_4$- and $C_6$-symmetric DSMs are then organized into topological universality classes, based on the monopole charge of Dirac points and the quantized Berry’s flux through generic $xy$-planes. The analysis of PWLs is presented in Sec. [VI]. Since Secs. [III], [IV], [V] are devoted to developing formalism for addressing bulk topology, general readers can consult the figures and skip to the experimentally relevant discussions in Sec. [VI]. In Sec. [VII] we describe non-perturbative, analytical solutions of surface-states for various DSMs. In Subsection [VIA] we discuss the spectra of surface-states, show-
ing the non-existence of helical Fermi arcs. The fermiology and spin-orbital textures of surface-states are addressed in Subsection [VIB]. We conclude by summarizing our main findings in Sec. VII. In Appendix A, we discuss the relationship between the surface-states Hamiltonians and the generators of Polyakov loops.

II. MODELS AND PHASE DIAGRAM

In this section, we consider a general class of $C_4$-symmetric DSMs. For clarity of presentation, we focus on the $D_{4h}$ point group, which supports $\mathcal{P}$ as a symmetry operation. This point group also possesses mirror symmetries with respect to the mutually orthogonal $xy$, $yz$, and $xz$ planes. In addition to the familiar $sp$- and $sd$-hybridized DSMs, we also describe a ME-DSM model. This will show (i) the topological universality of generic $xy$ planes, and (ii) the distinction between generic planes and $k_z=0, \pi$ mirror planes. We will work with the $O(5)$-vector

$$\mathcal{N}(k) = [t_p(k_z) \sin k_x, t_p(k_z) \sin k_y, t_{d,1}(k_z)(\cos k_x - \cos k_y), t_{d,2}(k_z) \sin k_x \sin k_y, t_s(\Delta - \sum_{j=1}^{3} \cos k_j)]$$

where $t_p(k_z)$, $t_s(k_z)$, $t_{d,1}(k_z)$, and $t_{d,2}(k_z)$ are four independent hopping parameters, and the dimensionless parameter $\Delta$ controls topological phase transitions. The $k_z$-dependence of hopping parameters determines whether the model preserves separate $\mathcal{P}$ and $\mathcal{T}$ symmetries. For $D_{4h}$ systems, $t_{d,1}(k_z) \neq t_{d,2}(k_z)$, as $(\cos k_x - \cos k_y)$ and $\sin k_x \sin k_y$ belong to different irreducible representations. By allowing them to mix, we can describe models for $C_{4h}$ point group, which supports $\mathcal{P}$ and mirror symmetry with respect to $xy$ planes. We employ the following representation of gamma matrices:

$$\begin{align*}
\Gamma_1 &= \tau_1 \otimes \sigma_1, \\
\Gamma_2 &= \tau_1 \otimes \sigma_2, \\
\Gamma_3 &= \tau_1 \otimes \sigma_3, \\
\Gamma_4 &= \tau_2 \otimes \sigma_0, \\
\Gamma_5 &= \tau_3 \otimes \sigma_0,
\end{align*}$$

where $\tau_j$ and $\sigma_j$ are $2 \times 2$ identity matrices. The two sets of Pauli matrices $\tau_j$ and $\sigma_j$ with $j=1,2,3$, respectively operate on the orbital and the spin indices.

$sp$-DSMs: The $\mathcal{P}$- and $\mathcal{T}$-preserving DSMs, arising from hybridizations between two orbitals of opposite parity and distinct rotation eigenvalues are described by an effective $SO(5)$ theory, commonly referred to as the $sp$-DSM model. This is obtained by setting $t_{d,1}(k_z) = t_{d,1}(k_z) \sin k_z, t_{d,2}(k_z) = t_{d,2}(k_z) \sin k_z$ in Eq. (6), leading to the $\mathcal{N}(k)$ of Eq. (1). Therefore, the Bloch Hamiltonian of $sp$-DSMs is given by

$$\mathcal{H}_{sp}(k) = t_p \sum_{j=1}^{2} \sin k_j \Gamma_j + t_{d,1} \sin k_z \cos k_x - \cos k_y \Gamma_3$$

The parity and the $C_4$ rotation eigenvalues of two orbitals are assumed to be $\{+1, e^{\pm i\theta_2}\}$ and $\{-1, e^{\pm i\theta_2}\}$, with $\theta_p = \frac{\pi}{4}(2p+1)$, $\theta_2 = \frac{\pi}{4}(2q+1)$, and $p,q \equiv 0 \mod 4$. The diagonal $\Gamma_5$ matrix labels distinct orbitals. Since the orbitals have opposite parity, $\Gamma_5$ also coincides with the parity operator $\mathcal{P}$. The separate $\mathcal{P}$, $\mathcal{T}$, and $\mathcal{C}_4$ symmetries lead to the following constraints: $\Gamma_5 \mathcal{H}_{sp}(k) \Gamma_5 = \mathcal{H}_{sp}(-k)$, $\Gamma_{31} \mathcal{H}_{sp}(-k) \Gamma_{31} = \mathcal{H}_{sp}(-k)$, and $\mathcal{C}_4 \mathcal{H}_{sp}(k) \mathcal{C}_4 = \mathcal{H}_{sp}(k')$, where $k_{\pm} = (k_x \pm i k_y)$, and $\mathcal{C}_4 = e^{i\theta} \Gamma_{34} e^{i\theta} \Gamma_{12}$, with $\theta = \frac{1}{4}(\theta_p + \theta_q) = \frac{\pi}{4}(p+q+1)$. By combining $\mathcal{P}$ and $\mathcal{T}$, the constraint of $\mathcal{PT}$ symmetry can be written as $\Gamma_{24} \mathcal{H}_{sp}(k) \Gamma_{24} = \mathcal{H}_{sp}(k)$.

$sd$-DSMs: The $SO(5)$ theory of DSMs, arising from hybridizations between two orbitals of same parity, but different rotation eigenvalues is known as the $sd$-DSM model. The Bloch Hamiltonian of $sd$-DSMs has the form

$$\mathcal{H}_{sd}(k) = t_p \sin k_z \sum_{j=1}^{2} \sin k_j \Gamma_j + t_{d,1} \sin k_z \cos k_x - \cos k_y \Gamma_3$$

obtained by setting $t_{d,1}(k_z) = t_p \sin k_z$, $t_{d,1}(k_z) = t_{d,1}$, and $t_{d,2}(k_z) = t_{d,2}$ in Eq. (6). The discrete symmetries are now implemented by $\mathcal{P} = 1$, $\mathcal{T} = i\Gamma_{24}$, $\mathcal{PT} = i\Gamma_5 \Gamma_{24} \mathcal{C}_4 = e^{i\theta} \Gamma_{34} e^{i\theta} \Gamma_{12}$. They impose the constraints: $\mathcal{H}_{sd}(k) = \mathcal{H}_{sd}(-k)$, $\Gamma_{24} \mathcal{H}_{sd}(-k) \Gamma_{24} = \mathcal{H}_{sd}(k)$, $\Gamma_{24} \mathcal{H}_{sd}(-k) \Gamma_{24} = \mathcal{H}_{sd}(k)$, and $\mathcal{C}_4 \mathcal{H}_{sd}(k) \mathcal{C}_4 = \mathcal{H}_{sd}(k')$, respectively.

Magneto-electric DSMs: By relaxing the requirements of separate $\mathcal{P}$ and $\mathcal{T}$ symmetries, we can construct models for $C_4$-symmetric, ME Dirac materials. An example of such ME Dirac models with orbitals of opposite parity is given by

$$\mathcal{H}_{ME}(k) = t_p \sum_{j=1}^{2} \sin k_j \Gamma_j + t_{d,1} \sin k_z \cos k_x - \cos k_y \Gamma_3$$

This is obtained from the $sp$-DSM model by setting $t_{d,1}(k_z) = t_{d,1}$ and $t_{d,2}(k_z) = t_{d,2}$. Since such materials lack separate $\mathcal{P}$ and $\mathcal{T}$ symmetries, $\Gamma_5 \mathcal{H}_{ME}(k) \Gamma_5 \neq \mathcal{H}_{ME}(-k)$ and $\Gamma_{31} \mathcal{H}_{ME}(-k) \Gamma_{31} \neq \mathcal{H}_{ME}(k)$. The same effective model can also be deduced from the $sd$-DSM model of Eq. (8), by setting $t_p(k_z) = t_p$. For this case, $\mathcal{H}_{ME}(k) \neq \mathcal{H}_{ME}(-k)$, $\Gamma_{24} \mathcal{H}_{ME}(-k) \Gamma_{24} \neq \mathcal{H}_{ME}(k)$. However, the combined $\mathcal{PT}$ and $\mathcal{C}_4$ symmetries remain unbroken, as $\Gamma_{24} \mathcal{H}_d(k) \Gamma_{24} = \mathcal{H}_d(k)$, and $\mathcal{C}_4 \mathcal{H}_d(k) \mathcal{C}_4 = \mathcal{H}_d(k')$. 

(8)

(9)
FIG. 1: Phase diagram of $C_4$-symmetric, Kramers-degenerate Dirac materials. The same structure of phase diagram is valid for the $sp$-, the $sd$-, and the magneto-electric Dirac semimetals, described by Eq. [8], Eq. [9], and Eq. [10], respectively. The Dirac semimetals (DSM) are gapless topological states, which interpolate between a trivial insulator (NI) and a topological insulator (TI). The topologically distinct phases are separated by quantum critical points (blue dots).

The universal structure of the phase diagram for all three types of Dirac materials is illustrated in Fig. 1. Akin to the WSMs, the DSMs also describe gapless, interpolating phases of matter, occurring between two topologically distinct insulating states. The non-trivial (trivial) insulator TI (NI) is realized in the parameter regime $|\Delta| < 1$, $|\Delta| > 3$. For $1 < \Delta < 3$, all components of $N(k)$ vanish at the Dirac points $k_D = (0, 0, \pm k_d)$, with $k_d = \cos^{-1}(\Delta - 2)$. For $-3 < \Delta < -1$, the Dirac points are located at $k_D = (\pi, \pi, \pm k'_d)$, with $k'_d = \cos^{-1}(\Delta + 2)$.

Notice the generic $xy$ planes (with $k_z \neq 0$, $\pi$, $\pm k_d$) of all three types of DSMs are described by the same effective model of two-dimensional insulators

$$\hat{H}_{2D}(k_x, k_y; k_z) = \hat{t}_p(\sin k_z \Gamma_1 + \sin k_y \Gamma_2) + \hat{t}_{d,1}(\cos k_x - \cos k_y)\Gamma_3 + \hat{t}_{d,2}(\sin k_x \sin k_y \Gamma_4) + t_s(\tilde{\Delta} - \sum_{j=1}^{2} \cos k_j)\Gamma_5,$$

(11)

where $\hat{t}_p = t_p(k_z)$, $\hat{t}_{d,j} = t_{d,j}(k_z)$ and $\tilde{\Delta} = \Delta - \cos k_x$. They break $T$ symmetry, while preserving $P$ and $C_4$ symmetries. When $1 < \Delta < 3$, and $|k_z| < k_D$, these insulators are topologically non-trivial, as they display band inversion between two $C_4$-symmetric, TRIM locations, $(k_x, k_y) = (0, 0)$, $(\pi, \pi)$, with respect to $\Gamma_5$. By contrast, the trivial $xy$ planes, lying outside the Dirac points $(|k_z| > k_D)$ do not exhibit band inversion. When $-3 < \Delta < -1$, the non-trivial (trivial) planes are found for $k'_d < |k_z| < \pi$ $(|k_z| < k'_d)$. The Dirac points describe topological quantum phase transitions between such trivial and non-trivial insulators. As long as $t_{d,1} \neq 0$, the two-fold-symmetric, TRIM locations $(k_x, k_y) = (\pi, 0), (0, \pi)$ remain gapped out and cannot participate in band inversion.

The crystalline-symmetry-enforced distinctions among three models of DSMs arise at the mirror planes located at $k_z = 0$, $\pi$. For the $sp$-DSM model, $N_3(k_z = 0, \pi) = 0$, $N_3(k_z = 0, \pi) = 0$ lead to the $O(2)$ symmetry, with respect to the mirror-operator $M_{xy} = \Gamma_{34}$. For the $sd$-DSM model, $N_1(k_z = 0, \pi) = 0$, $N_2(k_z = 0, \pi) = 0$ lead to $M_{xy} = \Gamma_{12}$. These two $P$ and $T$ preserving models respectively support mirror Chern numbers $\pm 1$ and $\pm 2$.

By contrast, the mirror planes of ME-DSM do not exhibit enhanced $O(2)$ symmetry, and all $xy$ planes are described by Eq. (11). The distinction between three models based on the $M_{xy}$ mirror symmetry manifests in the spectra of surface states, which will be presented in Sec. [VI]. In the following section, we describe the non-Abelian, Berry’s connections of generic planes using singular gauge.

III. SINGULAR BERRY’S CONNECTIONS

For convenience, we will label our conduction and valence bands with eigenvalues of $\Gamma_5$. For such choice of basis, the band inversion between $C_4$-symmetric TRIM points leads to singular form of Berry’s connections. The general form of diagonalizing matrix can be written as

$$U(k) = \begin{bmatrix} \cos \frac{\theta(k)}{2} g_+ (k) & i \sin \frac{\theta(k)}{2} u(k) g_- (k) \\ i \sin \frac{\theta(k)}{2} u(k) g_+ (k) & \cos \frac{\theta(k)}{2} g_- (k) \end{bmatrix} \in \frac{Spin(5)}{Spin(4)},$$

(12)

and $U^\dagger(k)\hat{H}(k)U(k) = |N(k)||\Gamma_5$. The first (last) two columns of $U$ correspond to the eigenfunctions of conduction (valence) bands. We have defined the polar angle $0 < \theta(k) < \pi$ on $S^1$ as $\cos[\theta(k)] = |N(k)|/|N(k)|$, and a four-component unit vector $\hat{n}_\mu = |N(k)|/[\sigma_0 + |N(k)|\sigma_0]$ with $\mu = 1, 2, 3, 4$. The SU(2) matrix $U(k) = |N(k)|/[\sigma_0 + |N(k)|\sigma_0]$ describes the hybridization matrix elements between two orbitals. The $Spin(4)$-matrix

$$G(k) = \begin{bmatrix} g_+(k) & 0 \\ 0 & g_- (k) \end{bmatrix},$$

(13)

describes gauge freedom in selecting band eigenfunctions, with $g_{\pm}(k) \in SU(2)$, and $|\Gamma_5, G(k)| = 0$. The six, block-diagonal matrices

$$\Gamma_{23} = \gamma_0 \otimes \sigma_1, \Gamma_{31} = \gamma_0 \otimes \sigma_2, \Gamma_{12} = \gamma_0 \otimes \sigma_3,$$

$$\Gamma_{14} = \gamma_3 \otimes \sigma_1, \Gamma_{24} = \gamma_3 \otimes \sigma_2, \Gamma_{34} = \gamma_3 \otimes \sigma_3,$$

(14)

act as the generators of the $Spin(4)$-group. These matrices can also be grouped into two triplets $\Sigma$ and $\Omega$:

$$\Sigma_j = \frac{1}{2}(1 + \Gamma_5)\Gamma_{j4}, \quad \Omega_j = -\frac{1}{2}(1 - \Gamma_5)\Gamma_{j4},$$

(15)

with $j = 1, 2, 3$, which generate two commuting $su(2)$ algebras for the conduction and the valence bands and provide a convenient description of intra-band, Berry’s connections. The off-diagonal $Spin(5)$ matrices

$$\Gamma_{15} = -\tau_2 \otimes \sigma_1, \Gamma_{25} = -\tau_2 \otimes \sigma_2, \Gamma_{35} = -\tau_2 \otimes \sigma_3,$$

$$\Gamma_{45} = \tau_1 \otimes \sigma_0$$

(16)

are useful for defining inter-band Berry’s connections.

The combined form of intra- and inter- band con-
nections can be obtained from the formula $A_j(k) = -iU^\dagger(k)\partial_j U(k)$. For $G(k) = 1_{4 \times 4}$, the intra-band, $Spin(4)$ Berry’s connections are given by

$$a_j(k) = 
\begin{bmatrix}
-i\sin^2 \frac{\theta(k)}{2} u(k) \partial_j u^\dagger(k) \\
0 \\
0 \\
-i\sin^2 \frac{\theta(k)}{2} u^\dagger(k) \partial_j u(k)
\end{bmatrix},
$$

$$= \frac{1}{2|N|(|N|+N_5)}(N_1 \partial_j N_2 - N_2 \partial_j N_1)\Gamma_{12} + (N_2 \partial_j N_3 - N_3 \partial_j N_2)\Gamma_{23} + (N_3 \partial_j N_1 - N_1 \partial_j N_3)\Gamma_{31} + \sum_{a=1}^3 (N_a \partial_j N_4 - N_4 \partial_j N_a)\Gamma_{a4}.
$$

For any general gauge choice, they obey inhomogeneous transformation $a_j \rightarrow \tilde{a}_j = G a_j G - iG^\dagger \partial_j G$. By operating with the projectors $P_{\pm} = (1 \pm \Gamma_5)/2$, we can extract the respective $SU(2)$ connections for conduction and valence bands. These connections exhibit singularities, when TRIM locations are mapped to the south pole of $S^4$, i.e., $\cos \theta = -1$. By performing a large gauge transformation, with

$$G(k) = \begin{pmatrix} u(k) & 0 \\ 0 & u^\dagger(k) \end{pmatrix},
$$

we can make the singularities to appear at TRIM locations, which are mapped to the north pole of $S^4$, with $\cos \theta = +1$. The transformed connections become

$$\tilde{a}_j(k) = 
\begin{bmatrix}
-i\cos^2 \frac{\theta(k)}{2} u^\dagger(k) \partial_j u(k) \\
0 \\
0 \\
i\cos^2 \frac{\theta(k)}{2} u(k) \partial_j u^\dagger(k)
\end{bmatrix},
$$

$$= \frac{1}{2|N|(|N|+N_5)}(N_1 \partial_j N_2 - N_2 \partial_j N_1)\Gamma_{12} + (N_2 \partial_j N_3 - N_3 \partial_j N_2)\Gamma_{23} + (N_3 \partial_j N_1 - N_1 \partial_j N_3)\Gamma_{31} + \sum_{a=1}^3 (N_a \partial_j N_4 - N_4 \partial_j N_a)\Gamma_{a4}.
$$

We can make the following observations, regarding the gauge choice for different phases in Fig. 1

1. Trivial insulators/NI: For the NI phase with $|\Delta| > 3$, all $xy$ planes are topologically trivial. When $\Delta > 3$ ($\Delta < -3$), both four-fold TRIM locations $(k_x, k_y) = (0, 0)$ and $(k_x, k_y) = (\pi, \pi)$ for all $xy$ planes get mapped to the north (south) pole of $S^4$. Consequently, Eq. (17) [Eq. (19)] describes the smooth gauge connections over the entire two-dimensional BZ, for $\Delta > 3$ ($\Delta < -3$).

2. Topological insulator/TI: For the TI phase, all $xy$ planes are topologically non-trivial, as $(k_x, k_y) = (0, 0)$ and $(k_x, k_y) = (\pi, \pi)$ points respectively map to the south and the north poles of $S^4$. Therefore, the connections of Eq. (17) and Eq. (19) will exhibit singularities, respectively at $(0, 0)$ and $(\pi, \pi)$. Hence, we encounter topological obstructions against defining smooth connections over the entire BZ two-torus.

3. DSMs: The same topological obstructions exist for the non-trivial $xy$ planes of DSMs.

Following Ref. [61], it is also possible to construct patchwise, smooth connections to cover the BZ. In the following section, we will work with singular connections to define quantized, Berry’s flux. For the non-trivial, planes, both types of singular connections lead to the same gauge-invariant, answer. For the trivial phases, we make the appropriate smooth gauge choice, while computing quantized flux with Abelian projected connections. If Eq. (17) [Eq. (19)] is employed for $\Delta < -3$ [$\Delta > 3$], the calculated flux will change by $\pm 4\pi$. The main reason behind this is the non-trivial properties of the hybridization matrix $u(k)$. For any arbitrary value of $k_z$, the $SU(2)$ matrices $u(k)$ and $u^\dagger(k)$ are the diagonalizing matrices of fictitious Chern insulators, which carry Chern numbers $\pm 2$. This can be seen by constructing the following Hopf maps: $u(k)\sigma_3 u^\dagger(k) = n_1(k) \cdot \sigma$, and $u^\dagger(k)\sigma_3 u(k) = n_2(k) \cdot \sigma$. The vectors $n_1(k)$ and $n_2(k)$ define orientations in $SU(2)$ color spaces, and implement the constraints of $C_n$ symmetry. Hence, they play important roles in gauge fixing procedure. Since they are independent of the band inversion parameter $\Delta$, they will be present for both trivial and non-trivial planes. By themselves, $u(k)$ and $u^\dagger(k)$ do not provide physical description of bulk topology of the $xy$ planes.

IV. ABELIAN PROJECTION AND QUANTIZED FLUX

A clear idea about the quantized flux can be obtained by performing Abelian gauge fixing with respect to the generators of $C_n$ operator. For stabilizing DSMs, the direction of nodal separation must coincide with the axis of $n$-fold rotation. Hence, the form of Bloch Hamiltonian is written in a global basis, labeled by parity and $C_n$ eigenvalues. In terms of $Spin(4)$ generators, the general form of $C_n$ is given by

$$C_n = e^{i\theta_p m_+ \cdot \Sigma} e^{i\theta_q m_- \cdot \Omega},
$$

where two, momentum-independent, three-component, unit vectors $\hat{m}_+$ and $\hat{m}_-$ specify global spin quantization axes for two, hybridizing orbitals. The diagonalization of $C_n$ corresponds to the choice $\hat{m}_1 = (0, 0, 1)$ and $\hat{m}_2 = (0, 0, 1)$, and

$$C_n = e^{i\theta_p \Sigma_+ e^{i\theta_q \Omega_3}} e^{i\theta_q \Sigma_4 e^{i\theta_p \Gamma_{12}}},
$$

with $\theta_+ = \frac{1}{2}(\theta_p + \theta_q) = \frac{\pi}{2}(p + q + 1)$, $\theta_- = \frac{1}{2}(\theta_p - \theta_q) = \frac{\pi}{2}(p - q)$. The specification of global spin quantization
axes for the hybridizing orbitals reduces the basis redundancy of band eigenfunctions from $SU(2) \times SU(2)$ to $U(1) \times U(1)$, leading to a modified coset space $S^3/\mathbb{Z}$ for the intra-band Berry’s connections, which admits second homotopy classification:

$$\pi_2 \left( \frac{Spin(4)}{U(1) \times U(1)} \right) = \pi_1(U(1) \times U(1)) = \mathbb{Z} \times \mathbb{Z}, \quad (22)$$

with $\mathbb{Z}$ being the group of integers. Consequently, the topologically non-trivial $xy$ planes and the Dirac points can be distinguished by a pair of integer invariants. This can be seen in the following manner.

The $C_n$ symmetry requires $C_n \bar{H}(k)C_n^\dagger = \bar{H}(k')$, which implements the constraint

$$[U^\dagger(k')C_nU(k), \Gamma_5] = 0, \quad (23)$$
on the diagonalizing matrix of Eq. (12). Here, the components of rotated wave vector are $k_\alpha' = k_\alpha \cos(2\pi n/3) - k_\beta \sin(2\pi n/3)$, $k_\beta' = k_\beta \cos(2\pi n/3) + k_\gamma \sin(2\pi n/3)$ and $k_\gamma' = k_\gamma$. The transformed operator $U^\dagger(k')C_nU(k)$ must be block-diagonal and an element of $Spin(4)$ group. The vanishing of block off-diagonal terms imply $u(k') = e^{i\theta\sigma_3}u(k)e^{-i\theta\sigma_3}$, leading to

$$N_1(k') = \cos(2\theta_+)N_1(k) + \sin(2\theta_+)N_2(k),$$

$$N_2(k') = \cos(2\theta_-)N_2(k) - \sin(2\theta_-)N_1(k),$$

$$N_3(k') = \cos(2\theta_-)N_3(k) + \sin(2\theta_-)N_4(k),$$

$$N_4(k') = \cos(2\theta_-)N_4(k) - \sin(2\theta_-)N_3(k),$$

$$N_5(k') = N_5(k), \quad (24)$$
as the transformation rules for the $O(5)$-vector $N(k)$. These are the basic criteria for constructing $C_n$ symmetric Bloch Hamiltonian. Furthermore, we obtain

$$U^\dagger(k')C_nU(k) = G(k)C_nG(k),$$

$$= \left[ g^\dagger_{\sigma_3}(k')e^{i\theta\sigma_3}g_{\sigma_3}(k) \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} g^\dagger_{\sigma_3}(k)e^{-i\theta\sigma_3}g_{\sigma_3}(k') \right]. \quad (25)$$

Therefore, under the $U(1) \times U(1)$ gauge transformations $g_{\pm}(k) = e^{i\alpha_{\pm}(k)\sigma_3}$, the form of $C_n$ remains unchanged: $U^\dagger(k')C_nU(k) = C_n$. For the gauge choice $G(k) = 1_{4 \times 4}$, the Abelian projected $U(1) \times U(1)$ connections can be obtained from Eq. (17), as $A_{j,Ab} = A_{j,12}^2 + A_{j,34}^2$, with $A_{j,12}^2 = \frac{1}{2}\text{Tr}[A_{j,\text{intra}}G_{12}]$ and $A_{j,34}^2 = \frac{1}{2}\text{Tr}[A_{j,\text{intra}}G_{34}]$. Hence, the explicit form of Abelian projected connections become

$$A_{j,Ab} = \frac{1}{2\mathcal{N}(|N| + N_5)} \left[ (N_1 \partial_1 N_2 - N_2 \partial_1 N_1) \Gamma_{12} + (N_3 \partial_1 N_4 - N_4 \partial_1 N_3) \Gamma_{34} \right]. \quad (26)$$

Under the $(U(1) \times U(1)$ gauge transformations $G(k) \rightarrow G(k') = \exp(i\alpha_{12}(k)\Gamma_{12}) \exp(i\alpha_{34}(k')\Gamma_{34})$, with $\alpha_{12}(k) = (\alpha_+(k) + \alpha_-(k))/2$, and $\alpha_{34}(k) = (\alpha_+(k) - \alpha_-(k))/2$, $A_{j,Ab}$ transforms as $A_{j,Ab} \rightarrow A_{j,Ab} + \alpha_{12}(k)\Gamma_{12} + \alpha_{34}(k)\Gamma_{34}$.

After some algebra, the Abelian projected field strength tensors $F_{ij}^{12} = \partial_i A_{j,12}^2 - \partial_j A_{i,12}^2$ and $F_{ij}^{34} = \partial_i A_{j,34}^2 - \partial_j A_{i,34}^2$ can be elegantly written as

$$F_{ij}^{12} = \sin(\theta_{12})[\partial_i \partial_j \phi_{12} - \partial_j \partial_i \phi_{12}], \quad (27)$$

$$F_{ij}^{34} = \sin(\theta_{34})[\partial_i \partial_j \phi_{34} - \partial_j \partial_i \phi_{34}]. \quad (28)$$

We have introduced two sets of spherical polar angles $(\theta_{12}(k), \phi_{12}(k))$ and $(\theta_{34}(k), \phi_{34}(k))$, such that

$$\tan[\phi_{12}(k)] = \frac{N_2(k)}{N_4(k)} \quad \text{and} \quad \tan[\phi_{34}(k)] = \frac{N_1(k)}{N_3(k)}, \quad (29)$$

and

$$\cos[\theta_{12}(k)] = \frac{N_2^2(k) + N_3^2(k)}{|N(k)| (|N(k)| + N_5(k))}, \quad (30)$$

$$\cos[\theta_{34}(k)] = \frac{N_2^2(k) + N_3^2(k)}{|N(k)| (|N(k)| + N_5(k))}. \quad (31)$$

These maps for projected field strength tensors determine the second homotopy classification of various planes. The quantized flux of $F_{ij}^{12}$ and $F_{ij}^{34}$ can only exist if BZ two-torus can wrap around the unit two spheres, defined by $(\theta_{12}(k), \phi_{12}(k))$ and $(\theta_{34}(k), \phi_{34}(k))$. For the generic $xy$ planes, the integer winding numbers or the relative Chern numbers are then given by

$$\mathcal{C}_{R,12}(k_z) = \frac{1}{2\pi} \int_{\gamma} dk_x dk_y F_{xy}^{12}(k), \quad (32)$$

$$\mathcal{C}_{R,34}(k_z) = \frac{1}{2\pi} \int_{\gamma} dk_x dk_y F_{xy}^{34}(k). \quad (33)$$

Notice that $\Phi_{xy}^{12}(k_z) = 2\pi \mathcal{C}_{R,12}(k_z)$ and $\Phi_{xy}^{34}(k_z) = 2\pi \mathcal{C}_{R,12}(k_z)$ describe the flux of Abelian fields $F^{12}$ and $F^{34}$, respectively. The topologically non-trivial (trivial) planes, lying between (outside) two Dirac points will support non-zero, relative Chern numbers. Since the relative Chern numbers jump at the Dirac points, they can be identified as $SO(5)$ monopoles, classified by two distinct integers $(\delta C_{R,12}, \delta C_{R,34})$.

For $C_4$-symmetric, linear DSMs described by Eq. (6), $\theta_{12}$ interpolates between 0 and $\pi$, leading to the skyrmion configuration for the unit vector

$$\hat{n}_{12} = (\sin \theta_{12} \cos \phi_{12}, \sin \theta_{12} \sin \phi_{12}, \cos \theta_{12}), \quad (34)$$

generic $xy$ planes, as shown in Fig. 2(a), In contrast to this, $\theta_{34}$ does not interpolate between 0 and $\pi$, and the unit vector

$$\hat{n}_{34} = (\sin \theta_{34} \cos \phi_{34}, \sin \theta_{34} \sin \phi_{34}, \cos \theta_{34}), \quad (35)$$
is topologically trivial, as shown in Fig. 2(b). Using these formulas, the relative Chern numbers for all $xy$ planes of the sp- and the ME DSMs are found to be

$$\mathcal{C}_{R,12}(k_z, \Delta) = -\Theta(k_{d,1} - k_z) \Theta(\Delta - 1) \Theta(3 - \Delta) -\Theta(k_z - k_{d,2}) \Theta(\pi - k_z) \Theta(-1 - \Delta) \Theta(3 + \Delta)$$
\[ \Delta = 2.0 - \pi - \pi/2 \]

\[ \langle \mathcal{C}_{R,12} \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_z \mathcal{C}_{R,12}(k_z), \]

\[ = -\frac{k_{d,1}}{\pi} \Theta(\Delta - 1) \Theta(3 + \Delta) - \left(1 - \frac{k_{d,2}}{\pi}\right) \Theta(-1 - \Delta) \times \Theta(3 + \Delta) - \Theta(1 - |\Delta|), \]

which is shown in Fig. 2(e). The topological properties of the generic \( xy \) planes and the Dirac points of \( sd \)-DSMs are identical to those of \( sp \) and ME-DSMs. The dis-

FIG. 2: Illustration of second homotopy classification of \( SO(5) \) connections with Abelian projected field strengths \( F^{12}_{ij}(k) \) and \( F^{34}_{ij}(k) \) of Eq. (27) and Eq. (28), respectively. (a) For a generic, topologically non-trivial \( xy \) plane, the three-component, unit vector \( \hat{n}_{12} \) of Eq. (34) displays skyrmion texture, with winding number \(-1\). (b) The unit vector \( \hat{n}_{34} \) of Eq. (35) does not exhibit such winding. (c) The relative Chern number [see Eq. (36)] or the quantized flux of \( F^{12}_{xy}(k) \) for the \( sp \) and the magneto-electric Dirac semimetals for \( \Delta = 2 \). (d) The vector plots of dipole configuration for Abelian projected magnetic fields \( B^{12}_{ij}(k) = \frac{1}{2} \epsilon_{ijl} F^{12}_{jl}(k) \). The momentum components are in units of \( \pi \). The Dirac points act as a pair of unit-strength, \( SO(5) \) monopole and anti-monopole, where \( \mathcal{C}_{R,12} \) jumps by \( \pm 1 \). (e) The average value of the relative Chern number \( \langle \mathcal{C}_{R,12} \rangle \) per \( xy \) plane, as a function of tuning parameter \( \Delta \).
constraint of $k_z = 0, \pi$ mirror planes can be taken into account with the following, modified formulas for the relative Chern numbers

$$\mathcal{C}_{R,12}(k_z, \Delta) = \begin{cases} -\Theta(k_z) & \text{for } k_z = 0 \\ \Theta(k_z) & \text{for } k_z = \pi \end{cases} \Theta(\Delta - 1) \Theta(3 - \Delta)$$

$$\mathcal{C}_{R,34}(k_z, \Delta) = \begin{cases} 0 & \text{for } k_z = 0 \\ -\Theta(1 - |\Delta|) & \text{for } k_z = \pi \end{cases} \Theta(3 - \Delta) \Theta(3 + \Delta).$$

The Abelian projections can also be performed for different choices of $G(k) \neq 1$. For any arbitrary $G(k)$, we can obtain the corresponding projected connections by taking trace of $\tilde{a}_j(k) = G^i(k) a_j G(k) - i G^i(k) \partial_j G(k)$ with $G^i(k) \Gamma^i_1 G(k)$ and $G^i(k) \Gamma^i_3 G(k)$. Using the relative Chern numbers and monopole charge, all crystalline-symmetry-allowed, stable linear DSMs can be grouped into different topological universality classes. Such organizing principles for $C_4$ and $C_6$ symmetric DSMs are shown in Tables I and II. The $C_3$-symmetric systems can also be addressed in a similar manner.

The outlined method of Abelian projection is physically appealing and sufficient for describing topology of four-band models, which are carefully constructed with detailed knowledge of global basis. This may not be very convenient for a quick analysis of a large tight-binding Hamiltonian of real materials. Therefore, in the next section, we describe a manifestly gauge invariant method for detecting quantized non-Abelian Berry’s flux, by computing PWL, defined by Eq. (5). This method is capable of identifying the magnitude of quantized flux.

V. PLANAR WILSON LOOPS

It is convenient to compute PWL by following the $C_4$ symmetric path $ABCD$ of Fig. 3(a). Without any loss of generality, we will choose the point $A$ with $(k_x, k_y) = (-k_0, -k_0)$ as our reference point. When the Kramers-degenerate wave functions are parallel transported between an initial point $k_i$ and a final point $k_f$, the matrix-valued, non-Abelian Berry’s phase is described by the Wilson line (or non-Abelian holonomy)

$$W_{i,f} = P \exp \left[ i \int_{l_i}^{l_f} \sum_{j=1}^{2} a_j(k(l)) \frac{dk_j}{dl} dl \right]$$

where $P$ denotes path ordering, and we have parametrized the line, joining two points as $k_i = k(l_i)$ and $k_f = k(l_f)$. Therefore, the PWL for path $ABCD$ can be obtained as the ordered product of four straight Wilson lines as

$$W_{ABCD}(k_0) = W_{A,B} W_{B,C} W_{C,D} W_{D,A}.$$  

Since $W_{ABCD}(k_0) \in Spin(4)$, we can parametrize it as

$$W_{ABCD}(k_0) = W_{ABCD,c}(k_0) W_{ABCD,v}(k_0)$$

and

$$W_{ABCD,c}(k_0) = \exp[i \theta_c(k_0) \mathbf{n}_c(k_0) \cdot \mathbf{\sigma}]$$

$$W_{ABCD,v}(k_0) = \exp[i \theta_v(k_0) \mathbf{n}_v(k_0) \cdot \mathbf{\sigma}].$$

| $(p, q)$ | Constraints | $\mathcal{C}_{R,12}$ | $\mathcal{C}_{R,34}$ | $N_{12}$ | $N_{34}$ |
|---------|-------------|-----------------|-----------------|---------|---------|
| $(1,3)$ | $p + q + 1 \equiv 1$ | $|p - q| = 2$ | $+1$ | $0$ | $\pm 1$ | $0$ |
| $(3,1)$ | $p + q + 1 \equiv 1$ | $|p - q| = 2$ | $-1$ | $0$ | $\pm 1$ | $0$ |
| $(0,2)$ | $p + q + 1 \equiv 3$ | $|p - q| = 2$ | $-1$ | $0$ | $\pm 1$ | $0$ |
| $(2,0)$ | $p + q + 1 \equiv 3$ | $|p - q| = 2$ | $-1$ | $0$ | $\pm 1$ | $0$ |

TABLE I: Topological universality classes for various $C_4$-symmetric Dirac semimetals, when the underlying point group is $D_{4h}$ or $C_{4v}$. The $C_4$ eigenvalues of hybridizing orbitals are given by $e^{\pm i\theta_p}$ and $e^{\pm i\theta_q}$, where $\theta_p = \frac{\pi}{4}(2p + 1)$, $\theta_q = \frac{\pi}{4}(2q + 1)$. Two integers $p$ and $q$ obey $p = 0, 1, 2, 3, 4, 5$ mod 6, $q = 0, 1, 2, 3, 4, 5$ mod 6, $p + q = 0$ mod 6, and $p + q + 1 \neq 0$ mod 6.

| $(p, q)$ | Constraints | $\mathcal{C}_{R,12}$ | $\mathcal{C}_{R,34}$ | $N_{12}$ | $N_{34}$ |
|---------|-------------|-----------------|-----------------|---------|---------|
| $(0,4)$ | $p + q + 1 \equiv 5$ | $|p - q| = 2$ | $-1$ | $0$ | $\pm 1$ | $0$ |
| $(3,1)$ | $p + q + 1 \equiv 5$ | $|p - q| = 2$ | $-1$ | $0$ | $\pm 1$ | $0$ |
| $(1,5)$ | $p + q + 1 \equiv 5$ | $|p - q| = 2$ | $-1$ | $0$ | $\pm 1$ | $0$ |
| $(2,4)$ | $p + q + 1 \equiv 5$ | $|p - q| = 2$ | $-1$ | $0$ | $\pm 1$ | $0$ |

TABLE II: Topological universality classes for various $C_6$-symmetric Dirac semimetals, when the underlying point group is $D_{6h}$ or $C_{6v}$. The $C_6$ eigenvalues of hybridizing orbitals are given by $e^{\pm i\theta_p}$ and $e^{\pm i\theta_q}$, where $\theta_p = \frac{\pi}{6}(2p + 1)$, $\theta_q = \frac{\pi}{6}(2q + 1)$. Two integers $p$ and $q$ obey $p = 0, 1, 2, 3, 4, 5$ mod 6, $q = 0, 1, 2, 3, 4, 5$ mod 6, $p - q = 0$ mod 6, and $p + q = 1 \neq 0$ mod 6.
Here, $W_{ABCD,c}(k_0) \in SU(2)$ and $W_{ABCD,c}(k_0) \in SU(2)$ are the PWLs for the respective $SU(2)$ connections of conduction and valence bands. Two angles $\theta_c(k_0)$ and $\theta_v(k_0)$ are gauge-invariant and two $O(3)$ unit vectors $\mathbf{n}_c(k_0)$ and $\mathbf{n}_v(k_0)$ define gauge-dependent orientations in color space.

From $\theta_{c/v}(k_0)$ we can construct other gauge-invariant quantities, such as (i) the eigenvalues of PWLs $\exp[\pm i \theta_{c/v}(k_0)]$, (ii) the trace of PWLs $\text{Tr}[W_{ABCD,c/v}(k_0) = 2 \cos[\theta_{c/v}(k_0)]$, and (iii) the Vandermonde determinant $D_{\text{V}}[W_{ABCD,c/v}(k_0)] = 2i \sin[\theta_{c/v}(k_0)]$ of PWLs. In gauge theory literature, $\text{Tr}[W_C]$ is the most widely studied observable. It is useful for detecting interpolation of $W_C$ between the center elements $\pm \sigma_0$ of $SU(2)$ group, leading to $\text{Tr}[W_C] = \pm 2$. When $\theta_{c,v} = 2\pi [2l \pm 1)\pi]$, with $l \in \mathbb{Z}$, $W_{C,c/v} = \sigma_0 [-\sigma_0]$. We determine both $\text{Tr}[W_{ABCD,c/v}]$ and $D_{\text{V}}[W_{ABCD,c/v}]$ to find $\theta_{c/v}$.

For Abelian connections of non-degenerate bands, the Stokes’s theorem directly relates $\theta_c$ and $\theta_v$ to the underlying Berry’s flux. As $k_0$ is tuned from 0 to $\pi$, $\theta_{c/v}(k_0)$ can interpolate between 0 and $2\pi$, with $l \in \mathbb{Z}$ being the Chern number, and a direct diagnostic of second homotopy classification. The windings of $\theta_c$ and $\theta_v$ for the non-Abelian connections also indicate the presence of chromo-magnetic flux, and non-trivial second homotopy classification. However, the interpretation of flux requires a non-Abelian generalization of Stokes’s theorem, and $\theta_{c,v}$ can be related to the surface-ordered, integrals of parallel-transported, non-Abelian curvatures

$$W_{xy} = P_s \exp \left[ i \int d^2k W_{A,O}^\dagger(k_x, k_y) f_{xy}(k_x, k_y) \right],$$

where $P_s$ denotes surface ordering, and $f_{xy}(k_x, k_y) = \partial_x a_y - \partial_y a_x + i(\sigma_y, a_y)$ corresponds to covariant curvatures. Here, $W_{A,O}(k_x, k_y)$ is the parallel transport operator, defined in Eq. (42), whose initial and final points are respectively located at $k = (-k_0, -k_0)$ and $k = (k_x, k_y)$ [see Fig. 3(a)]. There also exist alternative formulations of non-Abelian Stokes’s theorem, which remove surface ordering by expressing PWLs as coherent state path integral over the gauge group. Such analysis of PWLs will be presented elsewhere.

For all topologically non-trivial, $xy$ planes with $|k_z| < k_D$, $\theta_c(k_0)$ and $\theta_v(k_0)$ display 0 to $2\pi$ windings, as the size of loop $ABCD$ is systematically increased from 0 to $2\pi$, to cover the entire two-dimensional, BZ torus. This causes PWLs to interpolate between $Z_2$ centers of the respective $SU(2)$ subgroups. For some intermediate value of $0 < k_0 < \pi$, $\theta_{c,v}$ reaches $\pi$. Topologically trivial planes do not show such interpolations. In Fig. 3(b), we illustrate these behaviors for the occupied valence bands. All non-trivial planes of the $sp$- and the $ME$- DSMs and generic $xy$ planes of $sd$-DSMs (with $k_z \neq 0, \pi$) exhibit such windings. Only the mirror planes of $sd$-DSMs show 0 to $4\pi$ windings, as shown in Fig. 3(c). Consequently, the PWL reaches $-\sigma_0$ for two intermediate values of $k_0$. This is consistent with the mirror Chern numbers being $\pm 2$ for $sd$-DSMs.

It is not essential to work with $C_4$ symmetric loop, whose origin coincides with $k = (0, 0)$ or $(\pi, \pi)$. The topological properties of PWL should be independent of such choice. To show this, we have translated the origin of path $ABCD$ to $(k_x, k_y) = (1.2, 1.2)$. Under this shift, the detailed $k_0$ dependence of $\theta_{c,v}(k_0)$ is modified. However, the presence or absence of 0 to $2\pi$ windings, and the number of center interpolations remain unaffected, which are shown in Fig. 3(d). So far, we have worked with singular $Spin(4)$ connections, arising from labeling our basis with parity or $\Gamma_5$ eigenvalues. In the following subsection, we show the spectra of PWLs display invariance under $SO(5)$ or $Spin(5)$ gauge transformations. Therefore, it is capable of detecting bulk topology of $xy$ planes, irrespective of the choice of underlying global or local basis.

### A. Non-singular connections and $SO(5)$-invariance

Suppose the Bloch Hamiltonian is written in a different basis (arbitrary Bloch gauge), such that $\Psi'(k) = V^\dagger(k)\Psi(k)$, and $\hat{H}'(k) = V^\dagger(k)\hat{H}(k)V(k)$, where $V(k) \in Spin(5)$. For convenience, we will hold our $\Gamma$ matrices fixed and rotate the vector field as $N_i(k) \rightarrow N'_i(k) = R_{ij}N_j(k)$, where $R_{ij}$ is a $SO(5)$ rotation matrix. Consequently, the Bloch Hamiltonian acquires the form $\hat{H}'(k) = N'(k) \cdot \Gamma$. The spectra of conduction and valence bands and the locations of Dirac points remain unaffected, as $|\mathbf{N}(k)| = |\mathbf{N}'(k)|$. The new form of diagonalizing matrix $U'(k)$ can be obtained from Eq. (12) by replacing $N_i(k)$ with $N'_i(k)$. For $G(k) = \pm 1$, we arrive at new forms of intra-band, $Spin(4)$ connections

$$a'_j(k) = \frac{1}{2[|\mathbf{N}|(|\mathbf{N}| + \mathbf{N}_5)]} [(N''_j N'_2 - N'_2 N''_j) \Gamma_{12} + (N'_2 \partial_j N'_3 - N''_3 \partial_j N'_2) \Gamma_{23} + (N'_3 \partial_j N'_1 - N''_1 \partial_j N'_3) \Gamma_{31} + \sum_{a=1}^{3} (N'_a \partial_j N'_4 - N''_4 \partial_j N'_a) \Gamma_{4a}].$$

When $|\mathbf{V}(k), \Gamma_5| \neq 0$, the TRIM locations no longer map to south or north poles of $S^4$, as $|\mathbf{N}| \pm N'_5 \neq 0$, leading to non-singular, $Spin(4)$ connections. We have computed $\theta_{c,v}$ for four different orientations on $S^4$, defined according to

**Basis 0** : $V_0(k) = 1$, with $N'_j = N_j$ and $j = 1, ..., 5$;

**Basis 1** : $V_1(k) = \exp \left[ -i \frac{\alpha_1}{2} \Gamma_{45} \right]$, with $N'_4 = N_5 \sin \alpha_1$,

$N'_3 = -N_3 \sin \alpha_1 + N_5 \cos \alpha_1$, $\alpha_1 = \frac{\pi}{2}$,

$N'_j = N_j$ and $j = 1, 2, 3$;
The comparison among corresponding $\theta_c(k_0)$’s for $C_4$ symmetric loop $ABCD$ are shown in Fig. 4. We can clearly see the spectra of PWLs are invariant under $SO(3)$ gauge transformations. Therefore, PWL provides manifestly gauge invariant descriptions of bulk topology of DSMs, and can be used for tight-binding Hamiltonians of real materials. In the following section, we present analytical results for surface-states Hamiltonian to understand fermiology and spin-orbital textures.

VI. SURFACE STATES

Using the five-component vector $\mathbf{N}(k)$ of Eq. (6), the general form of $C_4$-symmetric DSMs can be written as

$$H(k) = t_p(k_z) \sin k_y \Gamma_1 + t_p(k_z) \sin k_y \Gamma_2$$

$$+ t_{d,1}(k_z)(\cos k_x - \cos k_y) \Gamma_3 + t_{d,2}(k_z) \sin k_x \sin k_y \Gamma_4$$

$$+ s(\Delta - \cos k_x - \cos k_y - \cos k_z) \Gamma_5.$$  \hspace{1cm} (48)

Here, the hopping functions have the form

$$t_j(k_z) = t_j^{(0)} + t_j^{(1)} \sin k_z,$$  \hspace{1cm} (49)

with $j \in \{p, d, 1\}$.

| $k_z$ | $\theta_c = \frac{N_j'}{j N_j}$ |
|-------|------------------|
| $|k_z|<|k_D|$ | ![Plot](a) |
| $|k_z|>|k_D|$ | ![Plot](b) |
| (0,0) | ![Plot](c) |
| (1.2, 1.2) | ![Plot](d) |

FIG. 3: (a) The $C_4$-symmetric path $ABCD$ for computing planar Wilson loops. (b) As we systematically increase the size of the loop by changing $k_0$ from 0 to $\pi$, $\theta_c(k_0)$ and $\theta_v(k_0)$ show 0 to $2\pi$ windings for all generic, topologically non-trivial $xy$ planes. The trivial planes do not support such windings. We are only showing the plots for the valence bands, as the conduction bands show identical behaviors. (c) When $1 < \Delta < 3$, the $k_z = 0$ mirror plane of $sd$-Dirac semimetals support 0 to $4\pi$ windings for $\theta_c(k_0)$ and $\theta_v(k_0)$. The same behavior is found for the $k_z = \pi$ plane, when $-3 < \Delta < -1$. This is consistent with the mirror Chern number being $\pm 2$. (d) The topological properties of $\theta_c$ do not depend on the choice of $C_4$-symmetric loop. We show the comparison between two square shaped loops, whose origins are respectively located at (0, 0) and (1, 2, 1, 2). The angles $\theta_c$ and $\theta_v$ are related to chromo-magnetic flux through non-Abelian Stokes’s theorem.
Spin basis are given by Eq. (47). The gauge invariant spectra

Therefore, the surface- conductance (n = +1) and valence (n = −1) bands on the (100) SBZ disperse as

\[ E_n(k_\perp) = \text{sgn}(n) |l_x(k_\perp)| \Theta(1 - |\lambda_{x,+}(k_\perp)|) \times \Theta(1 - |\lambda_{x,-}(k_\perp)|). \]  

The normalizability conditions restrict the surface-states to a finite region of the SBZ and their penetration depths are controlled by

\[ \lambda_\pm(k_\perp) = \frac{F_3 \pm \sqrt{F_3^2 + F_2^2 - F_1^2}}{F_1 + F_2}, \]

with

\[ F_1 = \sqrt{t_x^2(k_z) + t_{d,2}^2(k_z) \sin^2 k_y}, \quad F_2 = \sqrt{t_x^2 + t_{d,1}^2(k_z)} \]

\[ F_3 = \frac{1}{F_2} \left[ t_{d,1}^2(k_z) \cos k_y + t_x^2 (\Delta - \cos k_y - \cos k_z) \right]. \]  

Similar calculations for the (010) surface lead to

\[ \hat{H}_y(k_\perp) = t \left[ l_{y,1}(k_\perp)\sigma_1 + l_{y,3}(k_\perp)\sigma_3 \right] \times \Theta(1 - |\lambda_+(y, k_\perp)|) \Theta(1 - |\lambda_-(y, k_\perp)|), \]

with

\[ l_{y,1}(k_\perp) = t_p(k_z) \sin k_x, \]

\[ l_{y,3}(k_\perp) = t_s t_{d,1}(k_z) \left( \Delta - 2 \cos k_y - \cos k_z \right). \]

The expressions for \( \lambda_{y,\pm}(k_\perp) \) can be found from \( \lambda_{x,\pm}(k_\perp) \) by replacing \( k_y \) with \( k_x \).

The spectra of (100)-surface-states for various models of DSMs are shown in Fig. 3. We first consider the stacked Bernevig-Hughes-Zhang (BHZ) model with \( t_{d,1}(k_z) = t_{d,2}(k_z) = 0 \), and \( t_p(k_z) = t_\sigma \). The surface-states dispersions for this model become

\[ E_n(k_y, k_z) = \text{sgn}(n) |t_\sigma| \sin k_y |\Theta(1 - |\lambda_+(k_y, k_z)|) \times \Theta(1 - |\lambda_-(k_y, k_z)|), \]

with \( F_1 = t_\sigma^0, F_2 = t_\sigma, \) and \( F_3 = t_s (\Delta - \cos k_y - \cos k_z). \)

Clearly, this model supports helical edge states for all non-trivial \( xy \) planes, with \( |k_z| < k_d \). Since the helical edge states show band crossings at \( k_y = 0 \), the segment of \( k_z \) axis with \( |k_z| < k_d \), corresponds to the loci of two-fold, degenerate zero energy states or the helical Fermi arcs. This is shown in Fig. 5(a). At the images of bulk Dirac points, \( F_2 = F_3 = 0 \). Thus, the surface states are not normalizable at \( k_z = \pm k_d \). However, the generic \( xy \) planes of Kramers-degenerate DSMs only support gapped edge states, which can be seen from the surface state dispersions for the \( sp- \) (Fig. 5(b)), the \( sd- \) (Fig. 5(c)) and the ME- (Fig. 5(d)) DSMs, when \( k_z \neq 0 \). Consequently, the helical Fermi arcs cannot exist for Kramers-degenerate DSMs. Even though the images of bulk Dirac points do not support, normalizable zero energy surface states, all models support low lying excitations in the immediate vicinity of \( (k_y, k_z) = (0, \pm k_d) \),
FIG. 5: Illustrations of surface states dispersions on the (100) surface Brillouin zone, obtained from Eq. (53). (a) The decoupled Weyl semimetals model supports gapless, helical edge states for all topologically non-trivial $xy$ planes, leading to the loci of crossings between surface- conduction and valence bands or the helical Fermi arcs, along the $k_z$ axis, between the projections of bulk Dirac nodes. The surface states of (b) $sp$-Dirac semimetals, (c) $sd$-Dirac semimetals, and (d) magneto-electric Dirac semimetals. The generic, topologically non-trivial $xy$ planes of $sp$-, $sd$-, and magneto-electric Dirac semimetals support gapped, edge states. Only at the $k_z = 0, \pi$ mirror planes, the $sp$- and the $sd$- DSMs can support isolated band-crossings or zero energy states. Therefore, the Kramers-degenerate, stable Dirac semimetals cannot support helical Fermi arcs. The black dots represent the images of bulk-Dirac points, where the surface states are not normalizable and merge with bulk scattered states.

with universal form of spectra

$$E_n(k_y, \delta k_{z, \pm}) \approx n\sqrt{t^2_0(k_d) k_y^2 + \frac{t^2_0 t^2_{d1}(k_d)}{t^2_d + t^2_{d1}(k_d)}(\delta k_{z, \pm})^2},$$

(60)

where $\delta k_{z, \pm} = (k_z \pm k_d)$.

The mirror-symmetry related distinctions among three models of DSMs manifest along the $k_z = 0, \pi$ mirror lines of SBZ. When $1 < \Delta < 3 [-3 < \Delta < -1]$, the $sp$ DSM can support mirror Chern number $\pm 1$ for $k_z = 0, k_z = \pi$ plane, leading to a single, normalizable surface Dirac cone at $k_y = k_z = 0$ ($k_y = k_z = \pi$). Since the $sd$-DSMs possess mirror Chern number $\pm 2$, they support two normalizable, surface Dirac cones at $(k_y, k_z) = (\pm \cos^{-1}((\Delta - 1)/2), 0)$, when $1 < \Delta < 3$. No such normalizable zero modes exist for the ME-DSMs. Hence, the gapped edge states and nearly gapless, linear spectra in the immediate vicinity of projections of bulk Dirac points are the universal properties of surface-states.

B. Fermiology and spin-orbital textures

The fermiology of various models at small (large) chemical potential are illustrated in Fig. 6 [Fig. 7]. For the stacked BHZ model of $sp$-DSMs, at zero chemical potential ($\mu = 0$), the loci of zero energy states represent a pair of Fermi arcs, as shown in Fig. 6(a). They precisely terminate at the images of bulk Dirac points on the SBZ. At any finite chemical potential (say $\mu > 0$), for $|k_z| < k_d$, the surface conduction band will intersect the Fermi level at two values of $k_y$. This leads to a Kramers-pair of open Fermi surfaces, which will terminate at some $|k_y^*(\mu)| < k_d$ (see Fig. 7(a)). By systematically lowering the Fermi energy to zero, one can collapse the open Fermi surfaces to the actual Fermi arcs. This corresponds to a continuous evolution of open Fermi surfaces, without any quantum Lifshitz transitions.

Since all three types of Kramers-degenerate DSMs ($sp$, $sd$ and ME) host low lying excitations in the vicinity of $(k_y, k_z) = (0, \pm k_d)$, for small chemical potentials, they
The Fermi surfaces of the sp cones lead to closed Fermi pockets for the sp made at low chemical potentials, close to k not support Fermi arcs like the decoupled Weyl semimetals model. The distinction between different models can be seen in Fig. 6 through Fig. 7. All three types of Dirac semimetals support open Fermi surfaces around the projections of bulk Dirac points, as a universal feature. They do not support Fermi arcs like the decoupled Weyl semimetals model. The distinction between different models can be made at low chemical potentials, close to k_z = 0 mirror line, where the mirror-symmetry-protected, surface Dirac cones lead to closed Fermi pockets for the sp- and the sd- Dirac semimetals. As the surface chemical potential is gradually increased beyond model-dependent critical strengths, the Fermi surfaces of the sp-, the sd-, and the magneto-electric Dirac semimetals can undergo quantum Lifshitz transitions, leading to two, large, open Fermi surfaces, as shown in Fig. 7.

The universal structure at large Fermi energies emphasizes the topological non-triviality of all generic xy planes, lying between two bulk Dirac points.

lead to two, small, open Fermi surfaces around the projections of bulk Dirac points. The existence of such small, open Fermi pockets is a universal property of Kramers-degenerate DSMs, as can be seen in Fig. 6(b) through Fig. 6(d). In addition, the surface Dirac cones of the sp- and the sd- DSMs give rise to small, closed Fermi surfaces. The existence of such pockets are related to underlying mirror symmetries and have nothing to do with bulk Dirac points. Most of the SBZ remains gapped out.

When μ exceeds the maximum value of the spectral gap between surface- conduction and valence bands

$$|\mu^*| \approx \frac{t_{s,d}t_{d,1}}{t_{s,d}^2 + t_{d,1}^2} |\Delta - 3|,$$

the Fermi surfaces of sp-, sd- and ME- DSMs undergo quantum Lifshitz transitions, leading to two, large, open Fermi surfaces [see Fig. 7(b), Fig. 7(d)]. Therefore, for large μ, the gapped, edge states of most of the topologically, non-trivial, xy planes can contribute to the fermiology. Without knowing the underlying bulk topological

FIG. 6: The fermiology of surface states for various types of Dirac semimetals on the (100) surface Brillouin zone for small chemical potentials. (a) The true Fermi arcs of decoupled Weyl semimetals at zero, chemical potential: μ = 0. The fermiology of (b) the sp-Dirac semimetals with \((t_{p}^{(0)}, t_{d1}^{(1)}, t_{d2}^{(1)}) = (3/4, 1/2, 1/4)\), (c) the sd-Dirac semimetals, with \((t_{p}^{(1)}, t_{d1}^{(0)}, t_{d2}^{(0)}) = (3/4, 1/2, 1/4)\), and (d) the magneto-electric Dirac semimetals with \((t_{p}^{(0)}, t_{d1}^{(0)}, t_{d2}^{(0)}) = (3/4, 1/2, 1/4)\) for small chemical potentials. For all figures (Δ, t_z) = (2, 1), and the black dots represent the projections of the bulk Dirac points. Owing to the similarity of low energy spectra of surface states [Eq. (60)], all three types of Dirac semimetals support open Fermi surfaces around the projections of bulk Dirac points, as a universal feature. They do not support Fermi arcs like the decoupled Weyl semimetals model. The distinction between different models can be made at low chemical potentials, close to k_z = 0 mirror line, where the mirror-symmetry-protected, surface Dirac cones lead to closed Fermi pockets for the sp- and the sd- Dirac semimetals. As the surface chemical potential is gradually increased beyond model-dependent critical strengths, the Fermi surfaces of the sp-, the sd-, and the magneto-electric Dirac semimetals can undergo quantum Lifshitz transitions, leading to two, large, open Fermi surfaces, as shown in Fig. 7.

FIG. 7: The universal features of fermiology of various types of Dirac semimetals for large chemical potentials. The Kramers-pair of open Fermi surfaces for (a) the stacked Bernevig-Hughes-Zhang model, (b) the sp-, (c) the sd- , and (d) the magneto-electric Dirac semimetals, on the (100) surface Brillouin zone. The hopping parameters are same as in Fig. 6. The universal structure at large Fermi energies emphasizes the topological non-triviality of all generic xy planes, lying between two bulk Dirac points.
invariant for generic $xy$ planes, it is impossible to justify the existence of gapped states or their implications for fermiology.

The spin-orbital textures of surface states are determined by the $O(2)$ unit vector fields $\mathbf{l}_j(\mathbf{k}_\perp) = \mathbf{l}_j(\mathbf{k}_\perp)/||\mathbf{l}_j(\mathbf{k}_\perp)|| = [\cos(\gamma_j(\mathbf{k}_\perp)), \sin(\gamma_j(\mathbf{k}_\perp))]$, with $j = x, y$. The textures can be represented either by the vector-plots of $\mathbf{l}_x(\mathbf{k}_\perp)$ or the corresponding dual vector fields $\nabla_{\perp} \gamma_j(\mathbf{k}_\perp)$. In Fig. 8 we elucidate topological properties of $\mathbf{l}_x(\mathbf{k}_y,\mathbf{k}_z)$. While the plots of $\mathbf{l}_x(\mathbf{k}_y,\mathbf{k}_z)$ in Fig. 8(a) and Fig. 8(c) are useful for describing one-dimensional topology as a function of $\mathbf{k}_y$, for fixed values of $\mathbf{k}_z$, the plots of $\nabla_{\perp} \gamma_x(\mathbf{k}_\perp)$ in Fig. 8(d) and Fig. 8(f) provide a better idea about the nature of singularities. The normalizable states only exist within a restricted region of SBZ and the spin-polarized angle-resolved-photoemission-spectroscopy measurements can only access such normalizable, physical states. However, the overall topological properties of $\mathbf{l}_x(\mathbf{k}_\perp)$ provide valuable insight into the nature of underlying Berry’s connections and the bulk-boundary correspondence. We will briefly discuss this interesting topic in Appendix A.

**VII. CONCLUSIONS**

To summarize, we have developed rigorous second homotopy classification of stable, Kramers-degenerate DSMs, supporting bulk Dirac points along an $n$-fold axis of rotation. We have established the Dirac points as the source and sink of chromo-magnetic flux of $SO(5)$ Berry’s connections. This has been shown with the Abelian projected field strength tensors and the windings of gauge-invariant spectra of planar Wilson loops. The Abelian projected fields assign both magnitudes and directions.
for the quantized flux. In contrast to this, the spectra of PWLs can detect the magnitude of quantized flux. The PWLs can be efficiently used for addressing the bulk topology of all Dirac materials without relying on spectroscopic properties of surface-states. We also made detailed predictions for the fermiology and spin-orbital textures of nontrivial $xy$ planes for describing the spectroscopic features of surface-states. Our work shows the experimental search of gapless surface states, which is successful for detecting $Z_2$ topological insulators cannot work for describing topology of DSMs. Without the sharply defined bulk invariants one cannot justify the presence of gapped edge states. The detection of spin-orbital textures across the Lifshitz transitions of surface-states in future photo-emission experiments will provide valuable insight into the topology of Dirac semimetals.

**ACKNOWLEDGMENTS**

This work was supported by the National Science Foundation MRSEC program (DMR-1720139) at the Materials Research Center of Northwestern University, and the start up funds of P. G. provided by the Northwestern University. D.P. and J.M.R. acknowledge the Army Research Office under Grant No. W911NF-15-1-0017 for financial support and the DOD-HPCMP for computational resources.

**Appendix A: Surface-Hamiltonians vs. Polyakov loop Hamiltonians**

In this Appendix, we outline the close relationship between the surface-states Hamiltonians and the generators of straight Wilson lines or Polyakov loops. To address the nature of topological obstructions on a multiply connected manifold like BZ torus $T^d = S^1 \times S^1 \times \ldots \times S^1$, one often calculates Polyakov loops (PWLs) [24] along the principal axes $\hat{k}_j$ of BZ (non-contractible cycles of d-torus) with $j = 1, 2, \ldots, d$. The PL along the $j$-th axis

$$W_j(k_\perp) = P \exp \left[i \int_{-\pi}^{\pi} a_j(k_\perp, k_\perp) \, dk_j \right], \quad (A1)$$

describes map from the $(d-1)$-dimensional BZ (or $T^{d-1}$) to the non-Abelian gauge group $Spin(4)$, where $k_\perp$ corresponds to the transverse space components with $k_\parallel \cdot k_\perp = 0$. Under the $k_\perp$-dependent transformation $G(k_\perp) \in Spin(4)$, $W_j(k_\perp)$ transforms covariantly: $W_j(k_\perp) \rightarrow G(k)W_j(k_\perp)G(k_\perp)$. We can write a general representation

$$W_j(k_\perp) = e^{i \theta_{c,j}(k_\perp) \, n_{c,j}(k_\perp) \cdot \Sigma} e^{i \theta_{v,j}(k_\perp) \, n_{v,j}(k_\perp) \cdot \sigma} \Omega,$$

where the three-component, unit vectors $\mathbf{n}_{c,j}(k_\perp)$ and $\mathbf{n}_{v,j}(k_\perp)$ specify the orientations in $SU(2) \times SU(2)$-color space. Two gauge-invariant angles $\theta_{c,j}(k_\perp)$ control the eigenvalues of PLs or the Wannier centers. With a proper gauge choice, we can make the color vectors of PLs to coincide with $\mathbf{l}_j(k_\perp)$. Therefore, the generators of PLs are proportional to the surface-states Hamiltonians.

Usually 0 to 2$\pi$ windings of $\theta_{c,j}(k_\perp)$ and $\theta_{v,j}(k_\perp)$ are used as indicators of bulk topology and a diagnostic tools of bulk-boundary correspondence of zero-energy, surface-states. Such windings can be found in all non-trivial $xy$ planes of decoupled WSMs model, and the mirror planes of sp- and sd- DSMs. However, $\theta_{c,j}(k_y)$, $\theta_{v,j}(k_x)$ for the generic $xy$ planes of $O(5)$ models do not support 0 to 2$\pi$ windings, which are consistent with the absence of helical edge states. Hence, Wieder et al. performed topological classification of the generators of PL: Hermitian operators $H_{W,j}(k_\perp) = \mathbf{l}_j(k_\perp) \cdot \sigma$, defined over the entire, two-dimensional BZ [23]. The diagonalization of $H_{W,j}(k_\perp)$ or $W_j(k_\perp)$ reduces the $SU(2)$ gauge freedom down to $U(1)$, and such Abelian gauge choice is known as the “Polyakov gauge”. For non-trivial planes with fixed values of $k_\parallel$, $\theta_{c,j}(k_\perp)$, $\theta_{v,j}(k_\perp)$ shows 0 to 2$\pi$ windings, and $H_{W,j}$ describes one-dimensional, topological insulators. This can be clearly seen in Fig. 8(a)-Fig. 8(c). Since such windings are absent for $|k_\parallel| > k_d$, $H_{W,j}$ for trivial planes describes one-dimensional, trivial insulators. The nested Wilson loops [22] is a formal method for detecting the windings of $\gamma_{x/y}$.

At isolated locations of two-dimensional BZ, the eigenvalues of $H_{W,j}$ can become degenerate. At these locations, the Polyakov gauge fixing breaks down. Such gauge fixing singularities can be classified as vortex defects of $\gamma_x$, as illustrated in Fig. 8(d). For the ME DSM [Fig. 8(e)], only the projections of bulk Dirac points $k_\perp = (0, \pm k_d)$ manifest as the gauge-fixing singularities. They appear as a pair of vortex (orange dot) and anti-vortex (green dot), and the vanishing of net vorticity is a consequence of Nielsen-Ninomiya theorem.

As a consequence of mirror-symmetry, the sp- and the sd- DSMs can exhibit additional gauge-fixing singularities. For $1 < \Delta < 3$, Polyakov loop generator of sd-DSMs shows band crossings at $(k_y, k_z) = (\pm \cos^{-1}(\Delta - 1)/2), 0$, which host two, normalizable surface Dirac cones. Both of these are vortices and this is consistent with the mirror Chern number of $k_\parallel = 0$ plane being 2. However to maintain overall neutrality, the projections of bulk Dirac points act as anti-vortices. For the sp-DSMs, the Polyakov loop Hamiltonian displays band-touchings at all TRIM points $(k_y, k_z) = (0, 0), (\pi, 0), (0, \pi), (\pi, \pi)$, only the BZ center supports normalizable surface Dirac cone, when $1 < \Delta < 3$. The projections of Dirac points again appear as vortices.

Even though all gauge-fixing singularities do not lead to normalizable, zero-energy surface states, their topological properties (vorticity) are entangled. Irrespective of the detailed symmetries, the Abelian gauge fixing always breaks down at the Dirac points. This is a fun-
damental property of all non-Abelian monopoles. Being a bulk quantity, the Polyakov loop generator is always defined over restricted regions of SBZ, they can possess net vorticity and evade the constraints of Nielsen-Ninomiya theorem. Therefore, in spite of their close resemblances, the generators of Polyakov loop and the surface-states-Hamiltonians turn out to be topologically inequivalent.
