Part I: Staggered index and 3D winding number of Kramers-degenerate bands

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(Dated: September 22, 2022)

For three-dimensional (3D) crystalline insulators, preserving space-inversion (P) and time-reversal (T) symmetries, the third homotopy class of two-fold, Kramers-degenerate bands is described by a 3D winding number $n_{3,j} \in \mathbb{Z}$, where $j$ is the band index. It governs space group symmetry-protected, instanton or tunneling configurations of $SU(2)$ Berry connection, and the quantization of magneto-electric coefficient $\theta_j = n_{3,j}\pi$. We show that $|n_{3,j}|$ for realistic, \textit{ab initio} band structures can be identified from a staggered symmetry-indicator $\kappa_{AF,j} \in \mathbb{Z}$ and the gauge-invariant spectrum of $SU(2)$ Wilson loops. The procedure is elucidated for 4-band and 8-band tight-binding models and \textit{ab initio} band structure of Bi, which is a $Z_2$-trivial, higher-order, topological crystalline insulator. When the tunneling is protected by $C_{n\alpha}$ and $D_{n\alpha}$ point groups, the proposed method can also identify the signed winding number $n_{3,j}$. Our analysis distinguishes between magneto-electrically trivial ($\theta = 0$) and non-trivial ($\theta = 2s\pi$, with $s \neq 0$) topological crystalline insulators. In Part II, we demonstrate $\mathbb{Z}$-classification of $\theta$ by computing induced electric charge (Witten effect) on magnetic Dirac monopoles.

I. INTRODUCTION

Band structures of $\mathcal{P}\mathcal{T}$ symmetric materials are described by $2N \times 2N$ Bloch Hamiltonian matrix $\hat{H}(k) = \sum_{j=1}^{N} E_j(k)\hat{P}_j(k)$, where $N$, $E_j(k)$, $\hat{P}_j(k)$ respectively correspond to the total number, the energy eigenvalues, and the projection operators of two-fold Kramers-degenerate bands, and $k$ is the wave vector. Since $E_j(k)$ and $\hat{P}_j(k)$ remain unchanged by $U(2)$ gauge transformations of Bloch wave functions of Kramers pairs, $\hat{H}(k)$ describes maps from crystalline space groups to the coset space $(U(2)^N)_{\mathcal{P}\mathcal{T}}/(U(2))_0 = \mathbb{Z}_2$. The objective of topological band theory is to classify such maps with appropriate bulk invariants.\textsuperscript{1-14}

For three-dimensional (3D) insulators, a 4-component unit vector $\hat{d}_j(k)$ can be embedded in $\hat{P}_j(k)$, which wraps around the Brillouin zone (BZ) three-torus. Such instanton or tunneling configurations of $\hat{d}_j(k)$ can be classified by the third spherical homotopy group $\pi_3(S^3) = \mathbb{Z}$, leading to the 3D winding number $n_{3,j} \in \mathbb{Z}$. When $n_{3,j} \neq 0$, $U(2)$ Berry connection $A_j(k)$ inherits 3D tunneling configurations. Therefore, Wilson loop calculations can facilitate identification of $n_{3,j}$.

Exploiting rotation and mirror symmetries, $U(2)$ redundancy of Bloch wave functions can be reduced to $U(1) \times U(1)$ (or a smaller discrete sub-group). If such gauge-fixing procedure is properly implemented, the 3D winding number can be related to the Chern-Simons coefficient\textsuperscript{15,19}

$$CS_j = \frac{1}{8\pi^2} \int d^2k \ e^{abc} \text{Tr}[A_a,\partial_b A_{c,j}] + \frac{2i}{3} A_a, A_{b,j} \equiv n_{3,j}/2, \quad (1)$$

and the magneto-electric coefficient or axion angle

$$\theta_j = 2\pi CS_j = \pi n_{3,j}. \quad (2)$$

The primary goal of this work is to identify $|n_{3,j}|$ from symmetry analysis and the gauge-invariant spectrum of $SU(2)$ Wilson loops.

For concreteness, we will focus on materials, possessing $\mathcal{P}$ and $\mathcal{T}$ symmetries. For such systems, the numerical cost for Wilson loop calculations can be substantially reduced by symmetry analysis. The main idea is to perform a \textit{coarse classification} of bulk winding numbers, with fictitious “order parameter” type quantities, defined in momentum space on Miller hyper-cube, which are known as symmetry-indicators (SI).

The application of SIs for $\mathcal{P}$- and $\mathcal{T}$- symmetric topological insulators (TIs) was pioneered by Fu, Kane and Mele.\textsuperscript{3,4} They identified the strong, $Z_2$ topological index (STI) $(-1)^{v_{0,GS}} = (-1)^{n_{3,j}}$ from the product of parity eigenvalues at time-reversal-invariant-momentum (TRIM) points. The STI of a ground state, with $m$ occupied bands is given by $v_{0,GS} = \sum_{j=1}^{m} v_{0,j} \mod 2$. When an odd (even) number of $Z_2$-non-trivial bands are occupied, $v_{0,GS}$ identifies the ground state as a non-trivial (trivial) insulator.

By construction, $v_{0,j}$ cannot distinguish (i) between $n_{3,j} = 0$, and $n_{3,j} = 2s \neq 0$, and (ii) between different odd integers. Since the ground states of topological crystalline insulators (TCIs) support a combination of $Z_2$-trivial bands and an even number of $Z_2$-non-trivial bands, their analysis requires new methods.\textsuperscript{13,14} This led to generalization of SIs,\textsuperscript{30-33} $K$-theory analysis,\textsuperscript{34,35} and the analysis of Wilson loop spectrum or Wannier charge centers (WCC).\textsuperscript{36-42} However, we are not aware of any direct method for computing $n_{3,j}$ beyond the scope of $Z_2$-classification scheme.\textsuperscript{15,19} Therefore, it is difficult to predict whether TCIs can support quantized magneto-electric response with $\theta = 2s\pi$ and $s \neq 0$.

In this work, we will develop a comprehensive theoretical framework for computing $n_{3,j}$. We will introduce a staggered SI $\kappa_{AF,j} \in \mathbb{Z}$ for recognizing patterns of parity (and rotation) eigenvalues that lead to $n_{3,j} \neq 0$.\textsuperscript{i2,19}
Using $\kappa_{AF,j}$, the uniform $\mathbb{Z}_2$ index $\kappa_{1,j}$, and weak $\mathbb{Z}_2$-indices $(\kappa_{1,j}, \kappa_{2,j}, \kappa_{3,j})$, following three classes of non-trivial band topology will be identified:

(i) class A: 3D $\mathbb{Z}_2$-topology, and $n_{3,j} = (2s_j + 1)$;
(ii) class B: weak/2D $\mathbb{Z}_2$-topology, and $n_{3,j} = 0$;
(iii) class C: $\mathbb{Z}_2$-trivial, 3D topology, and $n_{3,j} = 2s_j$.

For these three classes of bands, $\kappa_{AF,j}$ respectively displays odd integer, zero, and even integer values. After performing coarse-classification with SIs, we will show that $n_{3,j}$ can be calculated from tunneling configurations of $SU(2)$ Berry flux (see illustration of Fig. 1). This will be accomplished with a joint analysis of WCC for high-symmetry planes and in-plane Wilson loops for high-symmetry planes.

The manuscript is organized as follows. In Sec. II, we introduce $\kappa_{AF,j}$ and discuss its relationship with $D$-dimensional winding number. In Sec. III, we analyze $O_h$-symmetry-protected, tunneling configurations, using an analytically tractable 4-band model. Contrasting properties of Wilson loops and surface Dirac fermions for three classes A, B, and C are demonstrated. In Sec. IV, we describe essential features of $D_{3d}$-symmetry-protected instantons by considering a 4-band model of rhombohedral systems. In Sec. V, we compute $|n_{3,j}|$ for ab initio band structure of Bi. In Sec. VI, we conclude with a brief discussion of our results. In Appendix A, we present calculate of signed winding numbers of an 8-band tight-binding model of Bi.

II. STAGGERED INDEX AND HOMOTOPY CLASSIFICATION

We begin with a physical perspective on SIs of parity eigenvalues for $D$-dimensional, simple cubic systems. The TRIM points of $D$-dimensional BZ (vertices of Miller hyper-cube) can be written as

$$Q^i = \frac{1}{2} \sum_{a=1}^{D} l_a^i \cdot b_a, \text{ with } i = 1, \ldots, 2^D,$$

where $b_a$ are reciprocal vectors, and $l_a^i = 0, 1$. The parity eigenvalues of $j$-th band are Ising variables $\delta_j^i = \pm 1$, located on the vertices of Miller-cube. Topological information encoded in $2N \times 2N$ diagonal matrices

$$P^i = \text{diag}[\delta_{1}^{0}, \ldots, \delta_{N}^{0}],$$

can be extracted by using matrix-valued “order parameters” or SIs.

The $\mathbb{Z}_2$ STIs of constituent bands are given by

$$\prod_{i} P^i = \text{diag}[(−1)^{v_{0,1}}, \ldots, (−1)^{v_{0,N}}],$$

$$(-1)^{v_{0,j}} = \prod_{i=1}^{2^D} \delta_j^i.$$  

The uniform or ferromagnetic indices are defined as

$$\kappa_1 = \frac{1}{2} \sum_{i=1}^{2^D} P^i = \text{diag}[\kappa_{1,1}, \ldots, \kappa_{1,N}],$$

$$\kappa_{1,j} = \frac{1}{2} \sum_{i=1}^{2^D} \delta_j^i,$$

and $\kappa_{1,j}$ can acquire $(2^D + 1)$ values

$$\kappa_{1,j} = 0, \pm 1, \pm 2, \ldots, \pm 2^{D−1}.$$

Due to the lack of band inversion, perfect ferromagnetic configurations [see Figs. 2(a) and 2(b)], describe topologically trivial bands, with $\kappa_{1,j} = \pm 2^{D−1}$. The uniform index of a ground state with $m$ occupied bands is defined by

$$\kappa_{1,GS} = \sum_{j=1}^{m} \kappa_{1,j} \mod 2^{D−1}, \text{ when } D > 1,$$

as it can be shifted by adding topologically trivial bands. Thus, $\kappa_{1,GS} = 0$, and $\kappa_{1,GS} = 2^{D−1} \times l$ with $l \in \mathbb{Z}$ correspond to topologically equivalent, trivial states, leading to the $\mathbb{Z}_2(2^{D−1})$-classification scheme for the ground state.

There exist

$$N_0 = \frac{2^{D_1}}{[2^{(D−1)}]!^2}$$
configurations, with $2^{D-1}$ positive, and $2^{D-1}$ negative parity eigenvalues, leading to $\kappa_{1,j} = 0$. We need new indicators to classify them. Notably, both topologically non-trivial configurations at $D = 1$ possess $\kappa_{1,j} = 0$. By focusing on maximally staggered, Néel configurations (see Fig. 2(c) and 2(d)), let us define

$$\kappa_{AF,j} = \frac{1}{2} \sum_{i=1}^{2^D} (-1)^{t_1^i + t_2^i + \cdots + t_D^i} \mathcal{P}^i,$$

$$\kappa_{AF,Gs} = \sum_{j=1}^{m} \kappa_{AF,j},$$

Akin to $\kappa_{1,j}$, $\kappa_{AF,j}$ can also acquire $(2^D + 1)$ distinct values

$$\kappa_{AF,j} = 0, \pm 1, \pm 2, \ldots, \pm 2^{D-1},$$

As trivial bands with perfect ferromagnetic configurations lead to $\kappa_{AF,j} = 0$, $\kappa_{AF,Gs} \neq 0$ cannot be deformed to 0 by adding topologically trivial bands. Therefore, the staggered index is a stable, $Z$-valued SI, which can be used for all inversion-symmetric systems. By construction, $(-1)^{\kappa_{1,j}} = (-1)^{\kappa_{AF,j}} = (-1)^{\nu_{0,j}}$, and $(-1)^{\kappa_{1,Gs}} = (-1)^{\kappa_{AF,Gs}} = (-1)^{\nu_{0,Gs}}$.

If our primary goal is to understand which configurations are capable of producing $D$-dimensional winding numbers, we can ignore $N_0$ configurations with $\kappa_{AF,j} = 0$. This can be seen from the explicit homotopy classification of minimal model

$$H(k) = \sum_{j=1}^{D+1} d_j(k) \Gamma_j = t_p \sum_{j=1}^{D} \sin k_j \Gamma_j$$

$$+ t_s [M - \Delta_1 \sum_{j=1}^{D} \cos k_j] \Gamma_{D+1},$$

of $D$-dimensional cubic topological insulators. Here $t_p$ and $t_s$ are hopping parameters, $(M, \Delta_1)$ are dimensionless tuning parameters, and $\Gamma_j$’s are $2^D \times 2^D$ mutually anti-commuting matrices, with $I \geq \lceil \frac{D+1}{2} \rceil$. The operation of $P$ is implemented as $\Gamma_{D+1} H(-k) \Gamma_{D+1} = H(k)$. Non-trivial $D$-dimensional band topology arises from instanton configurations of $O(D + 1)$ unit vector $\hat{d}(k) = d(k)/|d(k)|$, which are classified by the $D$-th spherical homotopy group $\pi_D(S^D) = Z$. The corresponding winding number

$$n_D = \frac{\Gamma(D+1)}{2 \pi} \int_{T^D} d^D k \ e_k \ \epsilon_{i_1 \ldots i_{D+1}} \hat{d}_{i_1} \partial_{i_2} \ldots \partial_D \hat{d}_{i_{D+1}},$$

counts how many times the BZ $D$-torus $T^D$ wraps around the unit-sphere $S^D$, and $\delta_n = \frac{\partial}{\partial t_n}$. The TRIM points support parity eigenvalues $\delta_{\pm} = \pm \text{sgn}[d_i(D+1)(Q')]$ for $2^{D-1}$-fold degenerate conduction (+) and valence (−) bands. When $t_s = 0$ and $t_p \neq 0$, they serve as hedgehogs of $O(D)$ unit vector, which can also be understood as merons of $O(D + 1)$ unit vector, with hedgehog charge

$$n_h = \left( \text{sgn}(t_p) \right)^D \left( -1 \right)^{t_1 + t_2 + \cdots + t_D}.$$  

By combining the hedgehog charge and parity eigenvalues, we arrive at

$$n_D = \mp \left( \text{sgn}(t_p) \right)^D \kappa_{AF,\pm}.$$  

Therefore, the homotopy analysis of intra-band Berry connection provides information about

$$n_{D,\pm} = \left( \text{sgn}(t_p) \right)^D \kappa_{AF,\pm} \mp n_D.$$  

Furthermore, we can rewrite $n_D$ as

$$n_D = n_{D-1}(k_i = \pi) - n_{D-1}(k_i = 0),$$

which describes the change of $(D - 1)$-dimensional winding number along $i$-th high-symmetry direction, supporting band inversion. This scheme of dimensional reduction provides an intuitive way to think about instanton configurations of vector fields and non-Abelian Berry connection [see Fig. 1]. The staggered index precisely keeps track of such tunneling configurations.

The dimensional reduction for non-Abelian Berry connection can be performed by Wilson loop along $j$-th axis

$$W_{j,-}(k_\perp) = P \exp \left[ i \int_{-\pi}^\pi A_{j,-}(k_j, k_\perp) dk_j \right],$$
TABLE I. Patterns of parity eigenvalues and symmetry indicators [see Eq. 28] for simple cubic systems, with $\Gamma = (0, 0, 0)$, $R = (1, 1, 1)$, $X = \{ (1, 0, 0), (0, 1, 0), (0, 0, 1) \}$, and $M = \{ (1, 1, 0), (0, 1, 1), (1, 0, 1) \}$. In Sec. III, we show that $O_h$-symmetry-protected tunneling configurations for simple cubic systems can be completely understood by considering the change of $SU(2)$ Berry flux along 4-fold or 3-fold axes. The staggered index tracks the bulk winding number, the number of normalizable surface Dirac cones, and the surface Hall conductivity of (001) and (111) surfaces.

| Parity eigenvalues $(\delta_\Gamma, \delta_R, \delta_X, \delta_M)$ | Symmetry indicators $(\kappa_{1, AF}; \nu_1, \nu_2, \nu_3)$ | Class |
|---------------------------------------------------------------|---------------------------------------------------------------|-------|
| 1. $(+1, +1, +1, +1)$ | $(+4; 0; 0, 0, 0)$ | Trivial |
| 2. $(-1, -1, +1, -1)$ | $(-4; 0; 0, 0, 0)$ | Trivial |
| 3. $(+1, +1, +1, +1)$ | $(+3; -1; 0, 0, 0)$ | A |
| 4. $(-1, -1, +1, -1)$ | $(-3; +1; 0, 0, 0)$ | A |
| 5. $(+1, -1, +1, +1)$ | $(+3; +1; 1, 1, 1)$ | A |
| 6. $(+1, -1, +1, -1)$ | $(-3; -1; 1, 1, 1)$ | A |
| 7. $(+1, +1, -1, +1)$ | $(+1; +3; 1, 1, 1)$ | A |
| 8. $(-1, +1, -1, +1)$ | $(-1; -3; 1, 1, 1)$ | A |
| 9. $(+1, +1, +1, -1)$ | $(-1; +3; 0, 0, 0)$ | A |
| 10. $(-1, -1, +1, +1)$ | $(+2; 0; 1, 1, 1)$ | B |
| 11. $(-1, -1, +1, +1)$ | $(-2; 0; 1, 1, 1)$ | B |
| 12. $(+1, -1, +1, +1)$ | $(+2; 1; 1, 1, 1)$ | C |
| 13. $(+1, +1, +1, +1)$ | $(-2; 1; 1, 1, 1)$ | C |
| 14. $(-1, -1, -1, +1)$ | $(+2; 0; 0, 0, 0)$ | C |
| 15. $(+1, +1, -1, -1)$ | $(-2; -1; 0, 0, 0)$ | C |
| 16. $(-1, -1, +1, -1)$ | $(+2; -1; 0, 0, 0)$ | C |

where P indicates path-ordering, and WCC are given by

$$\bar{\mathbf{j}}_-(\mathbf{k}_\perp) = \frac{1}{2\pi} \text{Im} \left[ \ln(W_{j,-}(\mathbf{k}_\perp)) \right].$$

When two TRIM points with identical (opposite) parity eigenvalues are joined by Wilson loop, $W_{j,-} \rightarrow \mathbb{1}$ ($-\mathbb{1}$) which are the center elements of gauge group (spin groups which are double covers of special orthogonal groups). The element $-\mathbb{1}$ corresponds to $\pi$ Berry phase or time-reversal polarization, and WCC describe interpolation between center elements as a function of $(D - 1)$- dimensional, transverse wave vector $\mathbf{k}_\perp$. In the following sections, we consider explicit examples of 3D simple cubic and rhombohedral models to elucidate the relationship between staggered index, bulk invariant and Wilson loops. To set the stage for such analysis, we provide simplified expressions of relevant SIs for some representative crystalline systems.

| Parity eigenvalues $(\delta_\Gamma, \delta_R, \delta_X, \delta_M)$ | Symmetry indicators $(\kappa_{1, AF}; \nu_1, \nu_2, \nu_3)$ | Class |
|---------------------------------------------------------------|---------------------------------------------------------------|-------|
| 1. $(+1, +1, +1)$ | $(+4; 0; 0, 0, 0)$ | Trivial |
| 2. $(-1, -1, -1)$ | $(-4; 0; 0, 0, 0)$ | Trivial |
| 3. $(+1, -1, -1)$ | $(+3; -1; 0, 0, 0)$ | A |
| 4. $(+1, -1, -1)$ | $(-3; +1; 0, 0, 0)$ | A |
| 5. $(+1, -1, -1)$ | $(+1; +3; 0, 0, 0)$ | A |
| 6. $(+1, -1, -1)$ | $(-1; +3; 0, 0, 0)$ | A |
| 7. $(+1, -1, -1)$ | $(0; +4; 0, 0, 0)$ | C |
| 8. $(-1, -1, -1)$ | $(0; -4; 0, 0, 0)$ | C |

TABLE II. Patterns of parity eigenvalues and symmetry indicators [see Eq. 29] for FCC crystals, with $\Gamma = (0, 0, 0)$, $X = \{ (1, 1, 0), (0, 1, 1) \}$. In contrast to simple cubic systems, tunneling of Berry flux for FCC systems occurs along (111) axis. Detailed analysis of tight-binding model and ab initio band structures of SnTe and PbTe will be presented in a separate work.

### A. Staggered index of selected 3D systems

At $D = 3$, there are total $2^8 = 256$ configurations of parity eigenvalues. The perfect ferromagnetic (trivial bands) and Néel configurations (bands with maximal winding numbers) are respectively characterized by

$$\langle \kappa_{1,j}; \kappa_{AF,j}, \nu_{1,j}, \nu_{2,j}, \nu_{3,j} \rangle = (\pm 4; 0, 0, 0, 0),$$

$$\langle \kappa_{1,j}; \kappa_{AF,j}, \nu_{1,j}, \nu_{2,j}, \nu_{3,j} \rangle = (0; \pm 4; 0, 0, 0),$$

and the weak $\mathbb{Z}_2$ indices $(\nu_{1,j}, \nu_{2,j}, \nu_{3,j})$ identify odd vs. even integer distinction of 2D winding numbers for (100), (010), and (001) planes, passing through the high-symmetry point $(l_1, l_2, l_3) = (1, 1, 1)$. For example,

$$(-1)^{\nu_{1,j}} = \delta_j^{(1,1,1)} \delta_j^{(1,1,0)} \delta_j^{(1,0,0)} \delta_j^{(1,0,1)},$$

$$\nu_{1,GS} = \sum_{j=1}^m \nu_{1,j} \mod 2.$$

Other $(2^8 - 4) = 252$ configurations of parity eigenvalues display imperfect ferromagnetic and staggered moments. Not all configurations are allowed by underlying crystal symmetries. For simple cubic systems (space groups 221 to 224) three X points (M) points support identical parity eigenvalue $\delta_X (\delta_M)$. Therefore, only 16
Parity eigenvalues \((\delta_T, \delta_L, \delta_X)\)  | Symmetry indicators \((\kappa_1; \kappa_{AF}; \nu_1, \nu_2, \nu_3)\)  | Class
---|---|---
1. \((+1,+1,+1,+1)\)  | \((+4;0,0,0)\)  | Trivial
2. \((-1,-1,-1,-1)\)  | \((-4;0,0,0)\)  | Trivial
3. \((-1,+1,+1,+1)\)  | \((+3;1,0,0)\)  | A
4. \((+1,-1,-1,-1)\)  | \((-3;1,0,0)\)  | A
5. \((-1,+1,+1,+1)\)  | \((+3;1,1,1)\)  | A
6. \((-1,-1,+1,+1)\)  | \((-3;-1;1,1)\)  | A
7. \((-1,+1,+1,-1)\)  | \((+1;3;1,1,1)\)  | A
8. \((-1,-1,+1,-1)\)  | \((-1;-3;1,1,1)\)  | A
9. \((+1,+1,+1,-1)\)  | \((+1;-3;0,0,0)\)  | A
10. \((-1,-1,-1,+1)\)  | \((-1;+3;0,0,0)\)  | A
11. \((-1,-1,+1,+1)\)  | \((+2;0;1,1,1)\)  | B
12. \((+1,+1,-1,-1)\)  | \((-2;0;1,1,1)\)  | B
13. \((-1,+1,-1,+1)\)  | \((0;+2;1,1,1)\)  | C
14. \((-1,-1,+1,-1)\)  | \((0;-2;1,1,1)\)  | C
15. \((-1,+1,+1,-1)\)  | \((0;-4;0,0,0)\)  | C
16. \((-1,+1,-1,+1)\)  | \((0;+4;0,0,0)\)  | C

TABLE III. Patterns of parity eigenvalues and symmetry indicators [see Eq. 30] for rhombohedral systems, with \(\Gamma = (0,0,0)\), \(T = (1,1,1)\), \(X = \{(1,1,0),(0,1,1),(1,0,1)\}\), and \(L = (1,0,0),(0,1,0),(0,0,1)\). In Sec. IV, we show that \(D_{\alpha\beta}\)-symmetry-protected tunneling configurations can be understood by considering the change of SU(2) Berry flux along 3-fold axis. The staggered index tracks the bulk winding number, the number of normalizable surface Dirac cones, along \(L\) and \(X\). The staggered index can be obtained using number, the number of normalizable surface Dirac cones, along \(L\) and \(X\). The staggered index can be obtained using

\[
\kappa_{1,j} = \frac{1}{2}(\delta_{T,j} + \delta_{R,j} + 3\delta_{X,j} + 3\delta_{M,j}),
\]

\[
\kappa_{AF,j} = \frac{1}{2}(\delta_{T,j} - \delta_{R,j} - 3\delta_{X,j} + 3\delta_{M,j}),
\]

\[
\nu_{1,j} = \nu_{2,j} = \nu_{3,j} = (1 - \delta_{R}\delta_{X}).
\]

Using \((\kappa_{1,j}; \kappa_{AF,j}; \nu_{1,j}, \nu_{2,j}, \nu_{3,j})\), we arrive at the coarse classification of Kramers-degenerate bands, listed in Table I. The SIs for primitive tetragonal and orthorhombic systems are easily obtained by distinguishing different \(X\) and \(M\) points. Consequently, additional configurations can be allowed. But the main idea of tracking 3D winding numbers with \(\kappa_{AF,j}\) remains unaffected.

For space groups 225-228, underlying FCC crystals lead to three \(X\) points and four \(L\) points. Therefore, only 8 configurations are allowed, which are listed in Table II, with SIs

\[
\kappa_{1,j} = \frac{1}{2}(\delta_{T,j} + 3\delta_{X,j} + 4\delta_{L,j}),
\]

\[
\kappa_{AF,j} = \frac{1}{2}(\delta_{T,j} + 3\delta_{X,j} - 4\delta_{L,j}),
\]

\[
\nu_{1,j} = \nu_{2,j} = \nu_{3,j} = 0.
\]

Importantly, FCC crystals do not support class B bands.

Rhombohedral systems are related to distorted FCC lattice. Due to rhombohedral distortion, (111) \(l\) point becomes inequivalent with other three \(L\) points, and is commonly known as the \(T\) point. Thus, rhombohedral systems allow 16 configurations of parity eigenvalues. The SIs are given by

\[
\kappa_{1,j} = (\delta_{T,j} + \delta_{T,j} + 3\delta_{X,j} + 3\delta_{L,j}),
\]

\[
\kappa_{AF,j} = (\delta_{T,j} - \delta_{T,j} + 3\delta_{X,j} - 3\delta_{L,j}),
\]

\[
\nu_{1,j} = \nu_{2,j} = \nu_{3,j} = \frac{1}{2}(1 - \delta_{T}\delta_{L}).
\]

and are listed in Table III. These SIs can be directly applied for analyzing ab initio band structures of materials like Bi, Sb, and Bi$_2$Se$_3$, when bands possess 3-fold rotation eigenvalues \(e^{\pm i\pi/3}\).

For bands with rotation eigenvalues \(e^{\pm i\pi}\), \(\Gamma\) and \(T\) points support \(n_{h}^\Gamma = \pm 3, n_{h}^T = \mp 3, n_{h}^X = \mp 1, n_{h}^L = \pm 1\) as hedgehog charge. Therefore, the staggered index of such bands is given by

\[
\kappa_{AF,j}^\pm = \frac{3}{2}(\delta_{T,j} - \delta_{T,j} + \delta_{L,j} - \delta_{X,j})
\]

Consequently, the staggered index of class A configurations 3-10 of Table III will be modified as

\[
\kappa_{AF,j}^\pm = -3, +3, +3, -3, -3, +3, +3, -3,
\]

respectively. Class C configurations 13 – 16 support

\[
\kappa_{AF}^\pm = -6, +6, 0, 0
\]

Hence, maximally staggered configurations with rotation eigenvalues \(e^{\pm i\pi/2}\) do not lead to 3D winding number. If the rotation data is not taken into account, Wilson loop calculations for 3-fold planes would guarantee that the correct magnitude of winding number is obtained.

For primitive hexagonal crystals, bands carrying rotation eigenvalues \(e^{\pm i\pi/3}\) and \(e^{\pm i\pi/2}\), the staggered index can be defined as

\[
\kappa_{AF,j}^{\pm/6} = \frac{3}{2}(\delta_{T,j} - \delta_{T,j} - 3\delta_{X,j} + 3\delta_{L,j}),
\]

\[
\kappa_{AF,j}^{\pm/2} = \frac{3}{2}(\delta_{T,j} - \delta_{T,j} - \delta_{X,j} + \delta_{L,j}).
\]

For simple toy models of bands with \(e^{\pm i\pi/3}\), \(K\) and \(H\) points can also participate in band inversion, and \(\kappa_{AF,j}^{\pm/6}\) should be modified by adding \((\delta_{K} - \delta_{H})\). Such examples can be found in Appendix A. Akin to rhombohedral systems, primitive hexagonal systems also support maximum staggered index \(\pm 6\).
III. SIMPLE CUBIC SYSTEMS AND $O_h$ INSTANTS

To understand topology of $O_h$ instanton configurations of Table I and $SU(2)$ Wilson loops, we consider a tight-binding model of two Kramers-degenerate bands, described by

$$H(k) = \sum_{j=1}^{5} d_j(k)\Gamma_j.$$  \hspace{1cm} (35)

Here $\Gamma_j$’s are $4 \times 4$ anti-commuting matrices, given explicitly as $\Gamma_{j=1,2,3} = \tau_1 \otimes \sigma_j$, $\Gamma_4 = \tau_2 \otimes \sigma_0$, and $\Gamma_5 = \tau_3 \otimes \sigma_0$, where $\sigma_{0,1,2,3}(\tau_{0,1,2,3})$ are $2 \times 2$ identity matrix and three Pauli matrices, operating on spin (orbital) index, respectively. Using $T_{1\alpha}$ and $A_{1\alpha}$ harmonics of $O_h$ point group, we define the following map

$$d_j(k) = t_p \sin k_j,$$

$$d_4(k) = M',$$

$$d_5(k) = t_s \left( M - \Delta_1 \sum_{j=1}^{3} \cos k_j - \Delta_2 \sum_{i<j=1}^{3} \cos k_i \cos k_j - \Delta_3 \prod_{j=1}^{3} \cos k_j \right),$$  \hspace{1cm} (36)

where $t_{p,s}$ are hopping parameters with units of energy, and $M, \Delta_1, \Delta_2, \Delta_3$ are dimensionless tuning parameters. For simplicity, the lattice constant has been set to unity. Parity and time-reversal symmetries are implemented as $P^\dagger H(-k)P = H(k)$, $T^\dagger H^*(-k)T = H(k)$, with $P = \Gamma_5$, $T = i\Gamma_{31} = i\tau_0 \otimes \sigma_2$, respectively, and $\Gamma_{ab} = [\Gamma_a, \Gamma_b]/(2i)$. The pseudo-scalar mass $M' \neq 0$ breaks $P$ and $T$ symmetries, but preserves the combined $PT$ symmetry, $\Gamma_{24} H^*(-k)\Gamma_{24} = H(k)$, and Kramers-degeneracy. When $M' \neq 0$, the 4-band model describes generic magneto-electric insulators, and $P$ and $T$ symmetric topological insulators are obtained for $M' = 0$. While computing Chern-Simons coefficient, it is convenient to use $M' \to 0^+$, as a suitable regulator of Dirac string singularities at TRIM locations.

All salient properties of topological insulators follow from the $O(4)$ vector $(d_1, d_2, d_5, d_5)$, and the $SU(2)$ matrix

$$u(k) = \hat{d}_5(k)\sigma_0 + i \sum_{j=1}^{3} \hat{d}_j(k)\sigma_j.$$  \hspace{1cm} (37)

At TRIM points parity eigenvalues of conduction $(\pm)$ and valence $(\mp)$ bands are given by $\pm \text{sgn}(d_5(Q^3))$ and $u(k)$ maps to $SU(2)$ center elements $\pm \sigma_0$. The 3D winding number is determined by

$$n_3 = \frac{1}{2\pi} \int_{T^3} d^3k \, e^{i\mathbf{k} \cdot \mathbf{a}} \delta_{\alpha \beta} \delta_{\alpha \beta} \partial_{\alpha} \partial_{\beta} \partial_{\alpha} \partial_{\beta} \partial_{\alpha} \partial_{\beta},$$

$$= \frac{1}{24\pi^2} \int_{T^3} d^3k \, e^{i\mathbf{k} \cdot \mathbf{a}} \, \text{sgn}(t_p) \, \kappa_{AF} = \pm 1, \pm 2, \pm 3, \pm 4.$$  \hspace{1cm} (38)

A representative phase diagram is shown in Fig. 3 for $M = +1, \Delta_3 = 2$. In Fig. 4, we display configurations of parity eigenvalues, SIs, and winding numbers for these phases.

As a consequence of cubic symmetry, all 4-fold symmetric planes exhibit $D_{4h}$ symmetry. Consequently, they manifest as crystal-symmetry-enforced defects of Bloch map, and the $O(4)$ vector reduces to $O(3)$ vector. Topology of such planes can be classified by the second homotopy group $\pi_2(S^2) = \mathbb{Z}$, and 2D winding numbers

$$\mathcal{C}_{m,ab}(\frac{1}{2} \epsilon_{j,k,j,k} = 0, \pi),$$

$$= \frac{1}{4\pi} \int_{T^2} d\mathbf{k}_s \, d\mathbf{k}_s \, \hat{d}(\mathbf{k}) \cdot (\partial_{\mathbf{k}_s} \hat{d}(\mathbf{k}) \times \partial_{\mathbf{k}_s} \hat{d}(\mathbf{k})).$$  \hspace{1cm} (40)

correspond to mirror Chern numbers, describing quantized, non-Abelian Berry flux through high-symmetry
Phases with 3D winding numbers \( n_{3,-} \neq 0 \), support distinct values of quantized, non-Abelian Berry flux \( 2\pi \epsilon_{R,ab} \) for \( k_j = 0, \pi \) planes. As a consequence of cubic symmetry, \( n_{3,-} \) is precisely related to the tunneling configuration of non-Abelian Berry flux, along three principal 4-fold axes

\[
n_{3,-} = \epsilon_{m,ab}(\frac{1}{2}\epsilon_{abj}k_j = \pi) - \epsilon_{m,ab}(\frac{1}{2}\epsilon_{abj}k_j = 0).
\]

For the present model, we can express mirror Chern numbers as

\[
\epsilon_{m,ab}(\frac{1}{2}\epsilon_{abj}k_j = 0) = \frac{1}{2}(2\delta_X - \delta_T - \delta_M),
\]

\[
\epsilon_{m,ab}(\frac{1}{2}\epsilon_{abj}k_j = \pi) = \frac{1}{2}(2\delta_M - \delta_R - \delta_X),
\]

leading to the exact relationship \( n_{3,-} = \kappa_{AF,--} \).

As weak topological insulators (Phase IV and Phase VIII) exhibit identical mirror Chern numbers for both \( k_j = 0, \pi \) planes, they do not support 3D tunneling configurations. In contrast to this, Phase II and Phase VI, which are commonly denoted as weak topological insulators, carry 3D winding numbers \( n_{3,-} = \pm 2 \). Since weak \( \mathbb{Z}_2 \) indices do not carry information regarding sign of mirror Chern numbers, they cannot address the presence or absence of even integer winding numbers.

Finally, Phase IX is of particular interest, as it supports tunneling configurations of even integer valued mirror Chern numbers for all 4-fold mirror planes. Also note
that even integer mirror Chern numbers occur for \(k_z = \pi\) planes of Phase V and \(k_z = 0\) planes of Phase VII, leading to strong topological insulators with higher winding number \(n_{3,-} = +3\).

Along any high-symmetry axis, joining \(Q^1\) and \(Q^2\), the \(O(4)\) vector \((d_1, d_2, d_3, d_4)\) reduces to \(O(2)\) vector, which can be classified by the fundamental group of circle \(\pi_1(S^1) = \mathbb{Z}\). Let us consider four high-symmetry lines parallel to the \(z\) axis, passing through \((k_x, k_y) = (0, 0), (\pi, 0), (0, \pi), (\pi, \pi)\). As these points correspond to TRIM locations of \((001)\) surface BZ, we will denote them as \(Q = \Gamma, X, Y, M\), respectively. The signed 1D winding numbers for high-symmetry axes are given by

\[
\begin{align*}
n_1(\Gamma) &= \frac{\text{sgn}(t_p)}{2}(\delta_X - \delta_Y), \\
n_1(X) &= n_1(\bar{Y}) = \frac{\text{sgn}(t_p)}{2}(\delta_M - \delta_X), \\
n_1(M) &= \frac{\text{sgn}(t_p)}{2}(\delta_R - \delta_M),
\end{align*}
\]

and these can be combined to write

\[
\begin{align*}
n_{3,-} &= [-n_1(\Gamma) + n_1(M) + n_1(X) + n_1(\bar{Y})] \\
&= \text{sgn}(t_p)\kappa_{AF,c-}.
\end{align*}
\]

When a high-symmetry axis supports non-trivial 1D winding number, it leads to normalizable 2-component, gapless Dirac fermions, under open boundary conditions along \((001)\) direction. In the presence of infinitesimally small regulator \(M' \to 0^+\), the surface Hamiltonians in the vicinity of TRIM locations are given by

\[
H(\bar{Q} + \delta k) \approx \text{sgn}(n_{1D}(\bar{Q})) \left[ \cos(Q_x)\delta k_y\sigma_1 - \cos(Q_y)\delta k_x\sigma_2 - \sigma_3M' \right].
\]

Therefore, the chirality of Dirac cone and the surface Hall conductivity is determined by \(\text{sgn}(n_{1D})\). While weak topological insulators (Phases IV and VIII) support Dirac cones at \((k_x, k_y) = (0, 0), (\pi, \pi)\), they come with opposite chirality, causing zero surface Hall conductivity. In contrast to this, Phases II and IX possess net surface Hall conductivity \(\pm e^2/h, \pm 2e^2/h\), respectively. Thus, the staggered index provides a precise description of bulk topology and bulk-boundary correspondence.

The importance of staggered index can be further emphasized by considering tunneling configurations of Berry flux along the 3-fold axis \((111)\) [see Fig. 5]. Phases II, IV, V, and IX respectively lead to 4, 0, 3, and 4 Dirac cones on \((111)\) surface. But the signed 1D winding number and \(\kappa_{AF,c}\) reveal that the Dirac cones for
Phase II at the center ($\bar{\Gamma}$) and the boundary of surface BZ ($M$) possess opposite chirality. Thus, the net surface Hall conductivity of Phase II remains fixed to $\pm e^2/h$, despite the presence of 4 Dirac cones.

These collective properties of $O(4)$ vector control topology of $SU(2)$ Berry connection and the regularized Chern-Simons coefficient

$$\mathcal{CS}_-(M' \rightarrow 0^+) = \frac{n_{3,-}}{2}. \quad (47)$$

For numerical tight-binding models of $ab$ initio band structure, the staggered index will provide a clear idea about the presence ($n_{3,j} \neq 0$) or absence ($n_{3,j} = 0$) of tunneling and the magnitude of winding number can be confirmed by Wilson loop calculations. Due to the $D_{4h}$ symmetry of mirror planes, bands carrying 3D winding number exhibit fully connected, gapless spectrum for $WCC$. Therefore, tunneling configurations along 4-fold axes of simple cubic systems can be fully characterized by gauge-invariant spectrum of $SU(2)$ Wilson loops.

Explicit calculations on analytically controlled 4-band model reveals the following features for Wilson loop $W_{111}$: (i) class A supports fully connected, gapless spectrum; (ii) class B shows gapped spectrum; and (iii) class C exhibits disconnected gapless spectrum. The number of gapless points are precisely counted by the number of non-trivial high-symmetry axes parallel to (111), or the staggered index [see Fig. 5]. The calculation of Berry flux for 3-fold planes has some subtleties, which are explained in the following sections.

**IV. RHOMBOHEDRAL SYSTEMS AND $D_{3d}$ INSTANTONS**

In Ref. 43, an elegant four-band, tight-binding model was proposed by Mao et al. for describing Bi$_2$Se$_3$. The 3D bulk Brillouin zone has the shape of a truncated octahedron, as shown in Fig. 6(a). The primitive reciprocal lattice vectors are given by

$$b_1 = (-1, -\sqrt{3}/3, b)g, \quad b_2 = (1, -\sqrt{3}/3, b)g,$$

$$b_3 = (0, 2\sqrt{3}/3, b)g, \quad (48)$$

where $b$ = 1/3 and $g$ = 2$\pi$, and the TRIM points are labeled by

$$\Gamma = (0, 0, 0), \quad L = \{(1, 0, 0), (0, 1, 0), (0, 0, 1)\},$$

$$T = (1, 1, 1), \quad X = \{(1, 1, 0), (0, 1, 1), (1, 0, 1)\}. \quad (49)$$

and the SIs follow from Eq. 30. The underlying point group corresponds to $D_{3d}$ and primary crystalline symmetries are: (i) 3-fold rotation about the [111] axis ($C_{3z}$); (ii) 2-fold rotations about [110], [101], and [011] axes (C$_2$); (iii) mirror symmetries for 2-fold planes $M_{110}$, $M_{010}$, and $M_{011}$; (iv) space-inversion symmetry ($P$).

The Bloch Hamiltonian has the form of Eq. 35 and $d(k)$ is given by

$$d_1(k) = -2A_{14} \sin w(\sin k_{a2} - \sin k_{a3}),$$

$$d_2(k) = -2B_{14} \sin w(\sin k_{g2} + \sin k_{g3}) - 2A_{14} \sin k_{a1} + \cos w(\sin k_{a2} + \sin k_{a3}),$$

$$d_3(k) = 2A_{12} \sum_{i=1}^{3} \sin k_{a2i},$$

$$d_4(k) = -2B_{12} \sum_{i=1}^{3} \sin k_{gi},$$

$$d_5(k) = 2A_{11} \sum_{i=1}^{3} \cos k_{a1} + 2B_{11} \sum_{i=1}^{3} \cos k_{gi} + m_{11},$$

$$ (50)$$

where $w = -2\pi/3$, $k_{a1} = k \cdot a$, and $k_{g1} = k \cdot g_1$, $a_1 = (a, 0, 0)$, $a_2 = (-\frac{a}{2}, \frac{\sqrt{3}a}{2}, 0)$, $a_3 = (-\frac{a}{2}, -\frac{\sqrt{3}a}{2}, 0)$, $g_1 = (0, \frac{\sqrt{3}}{c}, c)$, $g_2 = (-\frac{a}{2}, -\frac{\sqrt{3}a}{6}, c)$, and $g_3 = (\frac{a}{2}, \frac{\sqrt{3}a}{6}, c)$, and $c/a = b = 1/3$.

Under symmetry operations of $D_{3d}$ point group, ($d_1(k), d_2(k), d_3(k), d_4(k)$, and $d_5(k)$) respectively transform as $E_{u}$-doublet, $A_{2u}$-singlet, $A_{1u}$-singlet, and $A_{1g}$-singlet. The operations of $P$, $T$, $C_{3z}$, $C_{2x}$, and $M_{YZ}$ symmetries are respectively implemented with

$$\Gamma_5, \quad i\Gamma_{31}, \quad e^{i\pi/3\Gamma_{12}}, \quad i\Gamma_{14}, \quad \text{and} \quad \Gamma_5 \Gamma_{14} = \Gamma_{23}.$$

The presence of $A_{2u}$ harmonic is a natural consequence of crystalline symmetry. It does not affect symmetry-indicators and bulk winding numbers, and universal topological properties are captured by 4-component vector ($d_1, d_2, d_4, d_5$), and the $SU(2)$ matrix $u(k)$ = $d_5(k)\sigma_0$ + $i d_1(k)\sigma_1$ + $d_2(k)\sigma_2$ + $i d_4(k)\sigma_3$. Thus, Eq. 50 is a non-trivial example of 4-band model, where a homotopically non-trivial $O(4)$ vector remains embedded within $O(5)$ unit vector.

The current model is sufficient for capturing 14 out of 16 configurations (except $\kappa_{AF} = \pm 4$) of Table III and 3D winding numbers

$$n_{3,-} = -\text{sgn}(B_{12})\kappa_{AF,-} = \pm 1, \pm 2, \pm 3, \quad (51)$$

for $u(k)$. After regulating

$$d_3(k) \rightarrow d'_3(k) = M' + d_3(k),$$

the regularized Chern-Simons coefficient of valence bands is given by

$$\mathcal{CS}_-(M' \rightarrow 0^+) = \frac{n_{3,-}}{2}.$$ 

A representative phase diagram involving nine phases are shown in Fig. 6(c). A summary of SIs, bulk winding numbers, and Wilson loop analysis are presented in Fig. 7.
A. \textit{SU}(2) Wilson loops

Along all high-symmetry axes joining two TRIM points, the \textit{O}(5) vector reduces to different \textit{O}(2) vectors. For understanding the presence or absence of tunneling, we first consider 1D winding numbers for high-symmetry axes, which are parallel to \( \vec{z} \). Using hexagonal BZ, these lines can be identified as \( \Gamma T \equiv \Gamma A \) passing through \((k_x, k_y) = (0, 0)\), and three \( XL \equiv ML \) lines, respectively passing through \((2\pi, 0)\), \((\pi, \sqrt{3}\pi)\), and \((-\pi, \sqrt{3}\pi)\). The signed 1D winding numbers and 3D winding number can be related as

\[
\begin{align*}
n_1(\Gamma T) &= sgn(B_{12}) \frac{1}{2}(\delta_{T,-} - \delta_{T,+}), \\
n_1(XL) &= sgn(B_{12}) \frac{1}{2}(\delta_{L,-} - \delta_{X,-}), \\
n_1(\Gamma T) + 3n_1(XL) &= n_{3,-} = -sgn(B_{12})k_{AF,-}.
\end{align*}
\] (52)

When \( n_1 \) is non-trivial, \textit{SU}(2) Wilson loop \( W_{z,-}(k_x, k_y) \) displays gapless spectrum. The WCC spectrum \( \tilde{\epsilon}(k_x, k_y) \) for classes A (Phase V), B (Phase II), and C (Phase IV) are shown in Figs. 8(a)-8(c). As 3-fold planes lack mirror symmetry, class C bands exhibit disconnected, gapless spectrum (as emphasized for simple cubic systems). Therefore, the full connectivity of WCC is not an essential criterion to determine 3D winding number.

For 3-fold \( XY \) planes, \textit{O}(5) vector does not reduce to \textit{O}(3) vector. Thus, 2D winding numbers must be found from in-plane Wilson loops, defined as

\[
W_j(C) = P \exp \left[ i \oint \sum_{\alpha=1}^2 A_{\alpha,j}(k(l)) \frac{dk_\alpha}{dl} \right].
\] (53)

It describes \textit{SU}(2) Berry phase accrued by the \( j \)-th Kramers-degenerate band, when parallel-transported along a closed, non-intersecting curve \( C \), parameterized by \( k(l) \). As an element of \textit{SU}(2) group, \( W_j \) can be written as

\[
W_j(C) = \exp \left[ i\theta_j \hat{\Omega}_j \cdot \sigma \right].
\] (54)

By employing non-Abelian Stokes theorem, the gauge invariant angle \( \theta_j \) can be related to the magnitude of \textit{SU}(2) Berry flux enclosed by the loop \( C \). The in-plane loop will be calculated with 3-fold symmetry preserving contours [see Fig. 8(d)], and the area of the loop will be gradually increased from 0 to the area of hexagonal BZ. The magnitude of relative Chern number \( |\mathcal{C}_{3,XY;j}| \) is found from

\[
|\mathcal{C}_{3,XY;j}| = \frac{1}{2\pi} |\theta_j(k_0 = k_b) - \theta_j(k_0 = 0)|.
\] (55)

The computation of 2D winding numbers can be further simplified by taking advantage of crystalline symmetry, as explained in Figs. 8(e) and 8(f). The results for in-plane Wilson loops for Phases I, IV, and V are shown in Figs. 8(h)-8(i).

To further elaborate on important differences with simple cubic systems, we study \( YZ \) mirror planes, passing through \( k_z = 0, 2\pi \). For these planes \( d_2 = d_3 = 0 \), and we can compute mirror Chern numbers from the
FIG. 7. Tunneling configurations, symmetry-indicators, and bulk winding numbers for nine homotopically distinct, rhombohedral phases of Fig. 6(c). Parity eigenvalue +1 (−1) of valence bands is indicated by red (cyan) dot. All three types of band topology can be succinctly understood in terms of tunneling configurations of $C_3$-symmetry protected Berry flux through $XY$ planes. The $Z_2$ trivial (non-trivial) planes are colored blue (yellow).

$O(3)$ vector $(d_1, d_4, d_5)$. While class A bands support mirror Chern numbers

$$\mathcal{C}_{m, YZ}(k_x = 0) = \mathcal{C}_{m, YZ}(k_x = 2\pi) = \pm 1,$$

(56)
no tunneling occurs along 2-fold axis. In contrast to this, Class B and Class C bands do not possess any mirror Chern numbers. Thus, \( n_{3,x} \) cannot be identified from \( \xi_{m,YZ} \). With analytical and numerical insights gained for \( R3m \) instantons, in the following section we address topology of \textit{ab initio} band structure of Bi.

V. \textit{AB INITIO} BAND STRUCTURE OF BISMUTH

Though originally considered to be a topologically trivial system, refined symmetry-indicators show that the ground state admits both higher-order and rotational-symmetry-protected crystalline topology.\textsuperscript{36-52} Does this imply the existence of even integer 3D winding number? We will affirmatively answer this question with a combined analysis of \( \kappa_{AF} \) and \( C_3 \)-symmetry-protected tunneling configurations of non-Abelian Berry flux. This
understand these indicators one must consider the combined effects of bands 1 with fully occupied bands buckling. number of buckled honeycomb layers and the strength of tunneling configuration also underpins the diversity of topological phases that can be realized by varying the number of buckled honeycomb layers and the strength of bucking.\textsuperscript{53–62} We will directly analyze \textit{ab initio} data, as the sixteen band Liu-Allen model\textsuperscript{63} does not faithfully capture topological properties.\textsuperscript{64}

Since Bi is a rhombohedral system with space group \textit{R} \textit{3} \textit{m}\textsuperscript{65}, the BZ for primitive unit cell has the shape of truncated octahedron [see Fig. 6(a)]. The primitive reciprocal lattice vectors are given by Eq. 48, with \( b = 0.384919 \) and \( q = 1.36307 \text{\AA}^{-1} \).\textsuperscript{66} All density-functional theory (DFT) are carried out with Quantum Espresso software package.\textsuperscript{67–69} Exchange-correlation potentials employ Perdew-Burke-Ernzerhof (PBE) parametrization

| Band index \( i \) | \( G_{3\pi} \) eigenvalues | Parity eigenvalues \( (\delta_\Gamma, \delta_\Sigma, \delta_\Pi, \delta_\Omega) \) | \( Z_4 \) and weak \( Z_2 \) indices | Staggered index \( \kappa_{AF,i} \) | Class |
|-------------------|---------------------------|---------------------------------|---------------------------------|-----------------------------|-------|
| 1                 | \( e^{\pm i \frac{\pi}{3}} \) | \((+1, -1, -1, +1)\)           | \((0; 1, 1, 1)\)               | \(-2\)                      | C     |
| 2                 | \( e^{\pm i \frac{\pi}{3}} \) | \((-1, +1, +1, -1)\)           | \((0; 1, 1, 1)\)               | \(+2\)                      | C     |
| 3                 | \( e^{\pm i \frac{\pi}{3}} \) | \((-1, -1, +1, +1)\)           | \((+3; 1, 1, 1)\)              | \(+1\)                      | A     |
| 4                 | \( e^{\pm i \frac{\pi}{3}} \) | \((-1, +1, -1, -1)\)           | \((-2; 1, 1, 1)\)              | \(0\)                       | B     |
| 5                 | \( e^{\pm i \frac{\pi}{3}} \) | \((-1, -1, -1, -1)\)           | \((-3; 0, 0, 0)\)              | \(+3\)                      | A     |
| 6                 | \( e^{\pm i \frac{\pi}{3}} \) | \((-1, -1, +1, +1)\)           | \((+3; 0, 0, 0)\)              | \(-1\)                      | A     |
| 7                 | \( e^{\pm i \frac{\pi}{3}} \) | \((-1, +1, +1, -1)\)           | \((+2; 1, 1, 1)\)              | \(0\)                       | B     |
| 8                 | \( e^{\pm i \frac{\pi}{3}} \) | \((-1, +1, +1, -1)\)           | \((0; 1, 1, 1)\)               | \(-6\)                      | C     |
| 9                 | \( e^{\pm i \frac{\pi}{3}} \) | \((-1, -1, +1, +1)\)           | \((-1; 1, 1, 1)\)              | \(-3\)                      | A     |

FIG. 9. (a) Bulk band structure of Bi along high symmetry paths of primitive Brillouin zone (Fig. 6(a)) and light-red (cyan) dots denote parity eigenvalues +1 (-1) at time-reversal-invariant momentum points. Class A, Class B and Class C bands are respectively colored as green, purple, and blue. (b) Summary of symmetry data and indicators for various Kramers-degenerate bands of bismuth. According to Table III bands \( i = 1 \) through 9 have parity eigenvalue configuration numbers 14, 13, 5, 12, 4, 3, 11, 13, and 8, respectively. We have used Eq. 30, and 31 to account for the rotation eigenvalues. The hypothetical insulator with fully occupied bands 1 through 5 is a higher-order topological insulator, with ground state indicators given by Eq. 57. To understand these indicators one must consider the combined effects of bands 3, 4, and 5. If the chemical potential is placed between bands 1 and 2, the resulting insulator will exhibit class C topology. In contrast to this, all ground state indicators would vanish for the insulator obtained by placing the chemical potential between bands 2 and 3.
of generalized gradient approximation (GGA).\textsuperscript{70} All topological analysis are performed with Wannier90 and Z2pack software packages.\textsuperscript{39,40,71}

The bulk band structure for primitive unit cell and coarse topological classification are respectively shown in Fig. 9(a) and Fig. 9(b). Bismuth is a compensated semimetal with band 5 (6) producing hole pocket around \( \bar{T} \) point (electron pockets around \( \bar{L} \) points). This does not affect topology of constituent bands. The hypothetical gapped, ground state, involving occupied bands 1 through 5 is a higher-order, TCI, with ground state indicators

\[
(v_0, GS; \nu_1, GS; \nu_{AF, GS}; \nu_1, GS; \nu_2, GS; \nu_3, GS) = (0; -2; +4; 0, 0, 0).
\]  

(57)

Without considering rotation eigenvalues \( e^\pm i\pi \) of band 5, we would have found \( \nu_{AF, GS} = +2 \).

To guarantee the absence of non-trivial Wilson lines through generic locations of hexagonal planes, we have computed WCCs (\( \tilde{z}_i(k_x, k_y) \)) for different bands, which are displayed in Fig. 10. The results are in direct correspondence with those presented in Fig. 8(a)-8(c). Hence, we can conclude that class A, B, and C bands of Bi respectively support odd, zero, and even integer values of flux tunneling along \( C_3 \) axis. The calculation of mirror Chern numbers of occupied bands leads to

\[
\mathbf{c}_{m, YZ} = \text{diag}(0, 0, +1, 0, -1).
\]  

(58)

Again in full agreement with results of 4-band model, only class A bands are found to possess mirror Chern numbers. As bands 3 and 5 carry opposite mirror Chern numbers, the net mirror Chern number for the ground

---

**FIG. 10.** Spectra of \( SU(2) \) Wilson line \( W_{z,i}(k_x, k_y = 0) \) for different bands. In precise agreement with results from previous section, (i) Class A bands (3, 5, 6, and 9) exhibit fully connected, gapless spectrum; (ii) Class B bands (4 and 7) possesses gapped spectrum; (iii) Class C bands (1, 2, and 8) display disconnected, gapless spectrum. The number of gapless points for bands 3, 5 and 6 \textsuperscript{[9]} is one \textsuperscript{[3]} and located at the \( \bar{T} \) point [three \( M \) points] of surface Brillouin zone. The total number of gapless points for class C bands is 4 (\( \bar{T} \); and three \( M \) points of surface Brillouin zone). As indicated by the staggered index, class B bands lack tunneling of Berry flux.
respective colored light-blue, gold, and light-green.

FIG. 12. Tunneling configurations for occupied bands

The in-plane Wilson loop calculations for different bands also support classification based on $\kappa_{AF}$. Since the staggered index of bands 1 and 2 cancel each other, we only show the results for occupied bands 3, 4, and 5 in Fig. 11. Therefore, the ground state can carry net winding number $\pm 2$ or $\pm 4$. This uncertainty can be resolved by implementing detailed gauge fixing process for Berry connection. As Bi is ultimately a semimetal, we do not pursue such numerically expensive analysis for *ab initio* band structure. However, in Appendix A, we address signed winding number of an 8-band tight-binding model of Bi\(^{46}\), which can support ground state winding number 4.

VI. CONCLUSIONS

Our analysis for cubic model demonstrates the power of staggered index and Wilson loop for identifying signed 3D winding number for constituent Kramers degenerate bands and ground state. Similar analysis of tunneling of mirror Chern number can be carried out for tetragonal systems with space groups 83-88 ($C_{4h}$ instantons) and 123-142 ($D_{4h}$ instantons); hexagonal systems with space groups 174 ($C_{3h}$ instantants), 175-176 ($C_{6h}$ instantants), 187-190 ($D_{3h}$ instantants), 191-194 ($D_{6h}$ instantants). When high-symmetry planes lack mirror symmetry, the gauge-invariant magnitudes of relative Chern number and 3D winding number can be determined from Wilson loops, without detailed knowledge of underlying basis. Therefore, a combined analysis of staggered index, in-plane Wilson loop, and straight Wilson lines are sufficient to perform $\mathbb{Z}$ classification of 3D winding numbers for all $\mathcal{P}$ and $\mathcal{T}$ symmetric systems. While the application of staggered index requires $\mathcal{P}$ symmetry, Wilson loop calculations can be applied for addressing topology of $\mathcal{PT}$-preserving, magneto-electric systems.

Our work shows that states with $\kappa_{AF,GS} \neq 0$ can support $\sum_{j=1}^{m} n_{3,j} \neq 0$. Thus, we expect $\mathbb{Z}_2$-trivial, topological crystalline insulators with $\kappa_{AF,GS} \neq 0$ to possess quantized, magneto-electric coefficient $\theta = 2\pi$, with $s \in \mathbb{Z}$. The tight-binding model as well as *ab initio* band structure of bismuth support such conclusions. Can quantized topological response of such states be detected? To affirmatively answer this question, in Part II, we will probe topological response with magnetic monopole and vortices.

Appendix A: 8-band model of bismuth

The model is written using conventional unit cell, with BZ shown in. The Bloch Hamiltonian has the form

$$H(k) = \begin{bmatrix} H_{TBI}(k) + \epsilon & \delta M_{TB}(k) \\ \delta M_{TB}(k)^\dagger & H_{TBI}(k) - \epsilon \end{bmatrix},$$

where $H_{TBI}$ describe two 4-band, strong $\mathbb{Z}_2$ topological insulators, coupled by the hybridization matrix $M_{TB}$. The $\mathcal{P}$ and $C_{3z}$ for $H(k)$ follow as $\mathcal{P} = \mathcal{P}_1 \oplus \mathcal{P}_{1T}$ and $C_{3z} = C_{3z,1} \oplus C_{3z,1}$. For details of model parameters and explicit representations of symmetry operators, please consult the supplementary information of Ref. 46. Along the 3-fold axis all elements of $M_{TB}$ vanish as a consequence of $C_{3z}$ symmetry. The band structure and SIs are respectively shown in Fig. 12(a).

We will perform direct analysis of tunneling configurations of $SU(2) \times SU(2)$ Berry connection for occupied valence bands. From numerical results shown in Fig. 12(b), we find

$$\langle |\mathcal{C}_{3,XY;1}^\dagger |, |\mathcal{C}_{3,XY;2}\rangle(k_z = 0) = (0, 0), \quad \langle |\mathcal{C}_{3,XY;1}^\dagger |, |\mathcal{C}_{3,XY;2}\rangle(k_z = \pi) = (3, 1).$$

Thus, occupied bands 1 and 2 possess tunneling of Berry flux and the magnitudes of 3D winding numbers are

$$\langle n_{3,1}, n_{3,2} \rangle = (3, 1).$$

Hence, the ground state can exhibit net even integer winding number $\pm 4, \pm 2$.

To resolve uncertainties, we have performed explicit Abelian gauge-fixing in the following manner. We first regulate the Bloch Hamiltonian as

$$H(k) \rightarrow H(k) + \alpha \Gamma_{NA}$$

where the traceless diagonal matrix

$$\Gamma_{NA} = \sigma_3 \otimes \sigma_3 \otimes \sigma_3,$$
is a generator of Cartan sub-algebra for the coset space, which commutes with $C_{3,2}$. This separates Kramers-pairs by $|2\alpha|$ at the BZ center. Appealing to Abelian Stokes theorem, the signed Berry flux for non-degenerate bands can be calculated with Abelian in-plane Wilson loops or TKNNY formula for Chern number:

$$\mathcal{C}_{3,XY;j} = \lim_{\alpha \to 0} \frac{1}{2\pi} \int_{\Gamma 2} d^2k F_j(k) \quad (A7)$$

where

$$F_j(k) = \sum_{j \neq l} \text{Im} \left( \langle \psi_{1,k} | \partial_x \hat{H} | \psi_{j,k} \rangle \langle \psi_{j,k} | \partial_y \hat{H} | \psi_{l,k} \rangle / (E_{j,k} - E_{l,k})^2 \right).$$

By implementing this calculation, we find signed winding numbers

$$\langle \mathcal{C}_{3,XY;1}, \mathcal{C}_{3,XY;2} \rangle(k_x = 0) = (0, 0), \quad (A8)$$

$$\langle \mathcal{C}_{3,XY;1}, \mathcal{C}_{3,XY;2} \rangle(k_x = \pi) = (+3, +1), \quad (A9)$$

$$\langle n_{3,1}, n_{3,2} \rangle = (+3, +1). \quad (A10)$$

Therefore, the ground state of the 8-band model carries net 3D winding number +4.

If the hybridization matrix is switched off, the signed Berry flux and $N_3$ for 4-band models $H_{TB,I}(k)$ and $H_{TB,II}(k)$ can be calculated following Secs. III and IV. The decoupled model also leads to Eq. A10 for constituent occupied bands. This demonstrates the stability of third homotopy classification determined from the tunneling configurations of non-Abelian Berry flux.

**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. A part of this work was performed at the Aspen Center for Physics, which is supported by National Science Foundation grant PHY-1607611.

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