Bulk topological invariants in noninteracting point group symmetric insulators

Chen Fang,[1] Matthew J. Gilbert,[2,3] and B. Andrei Bernevig[1]

[1]*Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*

[2]*Department of Electrical and Computer Engineering, University of Illinois, Urbana, Illinois 61801, USA*

[3]*Micro and Nanotechnology Laboratory, University of Illinois, 208 N. Wright St, Urbana, Illinois 61801, USA*

(Received 1 August 2012; revised manuscript received 18 August 2012; published 10 September 2012)

We survey various quantized bulk physical observables in two- and three-dimensional topological band insulators invariant under translational symmetry and crystallographic point group symmetries (PGS). In two-dimensional insulators, we show that (i) the Chern number of a C_n-invariant insulator can be determined, up to a multiple of n, by evaluating the eigenvalues of symmetry operators at high-symmetry points in the Brillouin zone; (ii) the Chern number of a C_n-invariant insulator is also determined, up to a multiple of n, by the C_n eigenvalue of the Slater determinant of a noninteracting many-body system; and (iii) the Chern number vanishes in insulators with dihedral point groups D_n, and the quantized electric polarization is a topological invariant for these insulators. In three-dimensional insulators, we show that (i) only insulators with point groups C_n, C_{nh}, and S_n PGS can have nonzero 3D quantum Hall coefficient and (ii) only insulators with improper rotation symmetries can have quantized magnetoelectric polarization P_3 in the term $P_3\mathbf{E}\cdot\mathbf{B}$, the axion term in the electrodynamics of the insulator (medium).

DOI: 10.1103/PhysRevB.86.115112 PACS number(s): 73.20.At

I. INTRODUCTION

The study of novel topological phases of matter has become one of the most active fields in condensed matter physics. These phases are interesting because while deviating qualitatively from the conventional insulating phase, they cannot be described by any *local* order parameter in the Ginzberg-Landau-Wilson spontaneous symmetry breaking paradigm. Heuristically, the word "topological" implies the presence of some *global* property, i.e., contributed by all electrons in the system, that distinguishes this special phase. Such a property is usually marked by a global observable that takes different values in a topological phase and in the conventional insulating phase (normal phase) adiabatically continuable to the atomic limit. In addition, topological also implies that this global observable is quantized, or discretized, so that a topological phase cannot be adiabatically connected to the normal phase. Any quantized global observable characteristic to a topological phase is called a bulk topological invariant.

To date, topological phases have been identified in various systems, including those with intrinsic topological order (fractional quantum Hall states),[1–3] topological band insulators,[4–11] topological superconductors,[12–14] and topological semimetals.[15–19] The focus of this paper is on topological band insulators or, simply, topological insulators (TI). A typical and first example of TI is the integer quantum Hall state.[20] The bulk topological invariant of this state is the quantized Hall conductance, $\sigma_{xy} = ne^2/h$, where $n \in Z$, and its value remains fixed when the magnetic field and gate voltage change within a certain range, resulting in a series of plateaus. Thouless *et al.*[21] showed that the quantized Hall conductance is proportional to the Chern number (TKNN number) of a $U(1)$ bundle over the 2D magnetic Brillouin zone (BZ), first time linking a quantized physical quantity to a topological number previously studied in the context of algebraic topology and differential geometry. It was then realized that since the Chern number is well defined in any translationally invariant insulator regardless of the magnetic field, nonzero quantized Hall conductance can also appear *without* external magnetic field (or net magnetic flux). Insulators with nonzero Chern numbers are later dubbed Chern insulators (or quantum anomalous Hall insulators).[22] In general, the 2D Chern number of a translationally invariant insulator is given by[21]

$$C = \frac{i}{2\pi}\sum_{n\in\text{occ}}\int_{\text{BZ}}\epsilon_{ij}\partial_i\langle u_n(\mathbf{k})|\partial_j|u_n(\mathbf{k})\rangle d^2\mathbf{k}, \tag{1}$$

where $|u_n(\mathbf{k})\rangle$ is the Bloch wave function of the nth band at $\mathbf{k}$, and integral over Brillouin zone (BZ) should be replaced with the one over magnetic BZ if there is an external magnetic field. From Eq. (1), it is clear that the Chern number is a global quantity contributed by all occupied electrons in the system.

If on top of translational symmetry, there is time-reversal symmetry (TRS) in the system, then one can prove that the Chern number defined in Eq. (1) always vanishes, a case often referred to as trivial. In the absence of nonzero Chern number, the natural question then is what is the bulk topological invariant for this system, if any? The answer is obvious when the z component of the total spin, S^z_{tot} is conserved (commutes with the Hamiltonian), because in this case the two spin components are decoupled so that we can define the Chern numbers for spin up ($C_\uparrow$) and spin down ($C_\downarrow$), separately. Due to TRS, $C_\uparrow = -C_\downarrow$, hence the quantity

$$C_s = \tfrac{1}{2}(C_\uparrow - C_\downarrow) \tag{2}$$

is a nontrivial bulk topological invariant, also known as the spin Hall conductance[5,6] (when multiplied by $\hbar$). However, when S^z_{tot} is not conserved, the definition of the bulk topological invariant is not a simple extension of the Chern number. According to Fu and Kane,[7,8] the nontrivial topology in a 2D insulator with translational symmetry and TRS can be characterized by a Z_2 number, i.e., a quantity that takes only two values. The explicit expression of this Z_2 number is not given here but we point out that it is linked to a quantized physical quantity, namely, the change in the "time-reversal polarization" over half of the BZ. The Z_2 bulk topological

invariant thus defined can be generalized to 3D insulators with TRS,[8,23,24] where it is given by

$$P_3 = \frac{1}{16\pi^2}\int d^3k\epsilon_{ijk}\mathrm{Tr}\left[\left(\mathcal{F}_{ij} - \frac{2}{3}i\mathcal{A}_i\mathcal{A}_j\right)\mathcal{A}_k\right] \bmod 1. \tag{3}$$

In Eq. (3), we have defined the non-Abelian Berry connection

$$\mathcal{A}_i^{mn}(\mathbf{k}) = i\langle u_m(\mathbf{k})|\partial_i|u_n(\mathbf{k})\rangle, \tag{4}$$

where $|u_n(\mathbf{k})\rangle$ is the Bloch state and the non-Abelian Berry curvature or field strength

$$\mathcal{F}_{ij}(\mathbf{k}) = \partial_i\mathcal{A}_j - \partial_j\mathcal{A}_i + i[\mathcal{A}_i,\mathcal{A}_j]. \tag{5}$$

From Eq. (3), we can see that P_3 is a global quantity depending on the band structure of all occupied bands in the whole BZ. In 3D, P_3 has another physical meaning: it is the coefficient of the axion term of the electrodynamics of the insulator in the compact space (having periodic boundary conditions in all directions),[24,25]

$$H_{\mathrm{axion}} = P_3\mathbf{E}\cdot\mathbf{B}, \tag{6}$$

and is, in principle, measurable with electromagnetic induction experiments. In order for P_3 to be a Z_2 index (taking only two possible values), it must be quantized by some symmetry. In an insulator with no symmetry, P_3 defined in Eq. (3) is an arbitrary number between zero and unity; but TRS quantizes it to either zero or one half. Nontrivial Z_2 topological insulators in 2D and 3D have odd number of gapless Dirac edge and surface modes, respectively, as has been confirmed by experiments.[26–28] Other than the linear dispersion around the Dirac points, these surface/edge states distinguish themselves by the absence of backscattering.[10,29,30]

From these previous studies, we can see that symmetries of a system play a key role in the definition of its bulk topological invariants. TRS has a twofold effect: on one hand, it constrains the Chern number to be zero and, on the other hand, makes possible the definition of a new Z_2 number. An interesting question then is if we consider adding other symmetries to an insulator, will there be new bulk topological invariant(s) characteristic to the added symmetries? Answering this question on a general ground is not easy, because it takes a detailed study of the homotopy groups of continuous mappings from the d-dimensional BZ to a target space of projectors under the symmetry constraints. Along this line, Schnyder *et al.* gave a list of all bulk topological invariants for each of the ten classes of Hamiltonians in the presence/absence of TRS, particle-hole symmetry and chiral symmetry for $d = 1,2,3$.[14]

All the three symmetries considered in Ref. 14 are symmetries on internal degrees of freedom, which do not change the position or orbital character of an electron. Topological properties protected by these internal symmetries are in general robust against random factors such as disorder. Nevertheless, the requirement of TRS excludes a spectrum of interesting materials that have magnetism while particle-hole and chiral symmetries are not to be found in realistic normal insulators but only in superconductors or maybe optical lattices. Therefore it is desired to extend the study of topological invariants to systems with other symmetries. In condensed matter electronic systems, it is natural to consider the lattice symmetries in the classification of insulators, because of their universal existence in solids, nonmagnetic and magnetic. Along this line, Fu first studied possible new Z_2 index in 3D spinless TRS insulators with fourfold rotation symmetry;[31] Hughes *et al.*[32] and Turner *et al.*[33] independently developed theories for inversion symmetric topological insulators without TRS.

In 3D, there are 230 types of lattice symmetries in which the simplest, yet nontrivial, one is the inversion symmetry, which sends an electron at $\mathbf{r}$ to $-\mathbf{r}$ leaving its spin invariant. Insulators with inversion symmetry have been previously studied[32–34] and it is shown that this symmetry affects the topological properties in two ways. First, its existence places constraints on the values of bulk topological invariants such as the Chern number and the Z_2 number; in Ref. 32, it is shown that the parity (even or odd) of the Chern number is determined by the inversion eigenvalues of occupied bands at four inversion invariant $\mathbf{k}$ points in the BZ, regardless of the Bloch wave function at all other $\mathbf{k}$ points; the Z_2 number of a TI with TRS can also be determined by the inversion eigenvalues at all inversion invariant $\mathbf{k}$ points.[34] Second, inversion symmetry alone brings about new topological invariants *without* TRS. We have mentioned that P_3 is quantized to zero and one half by TRS, and Refs. 32 and 33 show that in the absence of TRS, P_3 is still quantized by inversion symmetry and is equal to, up to an integer, half of the winding number of the inversion sewing matrix (to be defined in Sec. II B).

In this paper, we study topological insulators subject to a more general class of lattice symmetries: crystallographic point group symmetries or, simply, point group symmetries (PGS).[31,35] Insulators with PGS are invariant under a certain set of rotations and reflections that leave at least one point fixed in space. In the language of crystallography, by only considering PGS and lattice translational symmetry, we restrict the discussion to insulators with symmorphic space groups. Simply speaking, in a symmorphic space group, there are only point group operations plus translations by lattice vectors, while the a general space group can contain combined operations of a point group operation followed by a translation of fractions of lattice vectors. We ask two questions regarding the relation between PGS and bulk topological invariants: (i) how does a given PGS constrain the value of a topological invariant such as the Chern number and (ii) can a given PGS give us new bulk topological invariants or quantized global quantities?

For 2D insulators, we answer these questions by an exhaustive discussion of all nine nontrivial PGS invariant insulators, divided into two types: those invariant under cyclic PGS $C_{n=2,3,4,6}$ and those under dihedral PGS $D_{n=1,2,3,4,6}$. For C_n-invariant insulators, we first show that the Chern number is determined by, or constrained by, the C_m eigenvalues of each occupied single-particle band at discrete high-symmetry points in BZ, where m evenly divides n. From there, we further prove that the Chern number modulo n is determined by the C_n eigenvalue of the *many-body* ground state, or Slater determinant in the noninteracting case. For D_n-invariant insulators, we prove that while the Chern number is constrained to zero, the electric polarization, or more strictly, the dislocation of the electronic charge center from the nearest lattice point, becomes a bulk topological invariant, the value of which is determined by eigenvalues of C_m.

In 3D, there are in total 31 nontrivial PGS, and instead of exercising an exhaustive study, we focus on establishing

TABLE I. Summary of major results regarding 2D PGS insulators. The index n always takes values of $n = 2,3,4,6$, and "eigenvalues at points of symmetry" is the short for C_m eigenvalues at C_m invariant points, where m divides n.

	Chern number	Electric polarization
C_n	Determined up to a multiple of n by egenvalues at points of symmetry	Nonzero Chern:undefined
		Zero Chern: quantized and determined by eigenvalues at points of symmetry
D_n	Zero	Quantized and determined by eigenvalues at points of symmetry

a link between the given PGS and the presence/absence of two experimentally interesting topological invariants: nonzero quantized 3D Hall conductance and quantized magnetoelectric coefficient P_3. We find that only C_n, C_{nh}, S_n PGS are compatible with nonzero Hall conductance while all other PGS lead to zero Hall conductance in all three components. Moreover, we prove that the sufficient and necessary condition for the quantization of P_3 (to zero and one half) is that the PGS contains at least one improper rotation, and $2P_3$ can be expressed as the winding number of the sewing matrix associated with that improper rotation symmetry. This excludes the following point groups from having quantized P_3: C_n, D_n, O, T, 11 distinct point groups in total. These major results are summarized in Table I for 2D and Table II for 3D cases.

The paper is organized as follows. In Sec. II, we introduce concepts and basic formulas constantly used throughout the paper, including a brief introduction to Hilbert space representations of crystallographic point groups in Sec. II A, definition and basic properties of the sewing matrix associated with a PGS operator in Sec. II B and the definition of basic properties of path-ordered loop integrals in BZ in Sec. II C. In Sec. III, we show how the Chern numbers in C_n-invariant 2D insulators can be determined by eigenvalues of symmetry operators at high-symmetry $\mathbf{k}$-points in Sec. III A, and how the Chern number in C_n-invariant 2D insulators can be determined by the C_n eigenvalue of the Slater determinant in Sec. III B. In Sec. IV, we show that D_n-invariant insulators have zero Chern number in Sec. IV A and that the electric polarizations are quantized thus being topological invariants and how to calculate them in Sec. IV B. We study 3D insulators with PGS in Sec. V, including the 3D quantum Hall effects in Sec. V A and quantization of 3D magnetoelectric coefficient P_3 in Sec. V B. In Sec. VI we conclude the work.

TABLE II. Summary of major results regarding 3D PGS insulators.

Hall conductance	Magnetoelectric polarization
Zero with $C_{nv}, D_n, D_{nh}, D_{2d,3d}, T, T_d, T_h, O, O_h$	Not-quantized with C_1, C_n, D_n, T, O
Quantized and determined by eigenvalues at points of symmetry with $C_1, C_n, C_{1v}, S_{2,4,6}$	Quantized with $C_{1v}, C_{nv}, C_{nh}, D_{nh}, D_{2d,3d}, S_{2,4,6}, T_d, T_h, O_h$

II. PRELIMINARIES

Before proceeding with the relevant background material, we briefly clarify the notations we use throughout the paper. When used as indices, the greek letters will always span the orbitals, while roman letters denote either the bands or spatial directions (x,y,z or k_x,k_y,k_z).

Throughout the text there are three different linear spaces in which operators are considered. First is the single-particle Hilbert space. The dimension of the single-particle Hilbert space is $N \times N_{\text{orb}}$, where N is the total number of sites and N_{orb} is the total number of atomic orbitals, including spin, per site. The second linear space is the orbital space. The dimension of the orbital space is N_{orb}. The third linear space is the occupied-band space. The dimension of this subspace is N_{occ}, where $N_{\text{occ}} < N_{\text{orb}}$ is the number of occupied bands. Summation of repeated indices is implicitly indicated when and only when the summation is over an index denoting the Cartesian coordinates: x,y,z and k_x,k_y,k_z.

A. Single-valued and double-valued representations of a double point group

In physics, properties of Hilbert space representations, i.e., operators, of symmetry group are more relevant than those of the group itself. For a point group, before defining the operators corresponding to each symmetry operation, it is necessary to extend the point group, G, to the double-point group G^D defined as $G^D = G \cup (\bar{E} * G)$, where $\bar{E}$ is a rotation of angle 2π about any axis in space, which satisfies $\bar{E}^2 = E$, and $\bar{E}g = g\bar{E}$ for $g \in G$. In this definition, we notice that a rotation of angle 2π is distinct from the identity element in G^D. All representations of G^D can be classified into single-valued representations and double-valued representations, in which $D(E) = D(\bar{E})$ and $D(E) = -D(\bar{E})$, respectively. In a physical system, the one-particle Hilbert space representation of G^D is a single-valued representation when the particle is spinless or of integer spin, and is a double-valued representation when the particle is of half odd integer spin. For example, of the C_n point group, if $\hat{C}_n$ is the single-particle operator for the n-fold rotation (and we will use a hat to denote operators in the single-particle Hilbert space), then we have $\hat{C}_n^n = \hat{I}$ if the particle is spinless or of integer spin, and $\hat{C}_n^n = -\hat{I}$ if the particle is of half odd integer spin, where $\hat{I}$ is the identity operator. To put the relations in a single equation: $\hat{C}_n^n = (-1)^F \hat{I}$, where F is two times the total spin of the particle.

B. Sewing matrix associated with a point group symmetry

It is assumed that our system is defined on a lattice, has translational invariance, and is noninteracting:

$$\hat{H} = \sum_{\mathbf{k}\in \text{BZ}} \hat{h}(\mathbf{k}) \equiv \sum_{\alpha,\beta,\mathbf{k}\in \text{BZ}} \tilde{H}^{\alpha\beta}(\mathbf{k}) c_\alpha^\dagger(\mathbf{k}) c_\beta(\mathbf{k}), \qquad (7)$$

where α,β denote the orbitals within a unit cell. When we say a Hamiltonian is invariant under point group G, we mean given

$R \in G$, there is

$$\hat{R}\hat{h}(\mathbf{k}) = \hat{h}(R\mathbf{k})\hat{R}, \tag{8}$$

where $R\mathbf{k}$ is the transformed wave vector $\mathbf{k}$ under R. For example, if R is an n-fold rotation C_n about z axis, $C_n\mathbf{k} = (k_x \cos(2\pi/n) - k_y \sin(2\pi/n), k_x \sin(2\pi/n) + k_y \cos(2\pi/n), k_z)$; if R is a mirror reflection about the xy plane M_{xy}, $M_{xy}\mathbf{k} = (k_x, k_y, -k_z)$.

At each $\mathbf{k}$, the eigenstates of $\hat{h}(\mathbf{k})$ are called the Bloch states, whose annihilation operators $\gamma_n(\mathbf{k})$'s satisfy

$$[\gamma_n(\mathbf{k}), \hat{h}(\mathbf{k})] = E_n(\mathbf{k})\gamma_n(\mathbf{k}), \tag{9}$$

where $n = 1, \ldots, N_{\text{orb}}$ is the band index. Then one can arrange γ_n in the ascending order of $E_n(\mathbf{k})$, such that for a fully gapped insulator, we have $E_n(\mathbf{k}) < E_f$ for $n < N_{\text{occ}} \leqslant N_{\text{orb}}$ for all $\mathbf{k} \in$ BZ. Combining Eqs. (8) and (9), we have

$$[\hat{R}\gamma_n(\mathbf{k})\hat{R}^{-1}, \hat{h}(R\mathbf{k})] = E_n(\mathbf{k}). \tag{10}$$

This equation shows that $\hat{R}\gamma_n(\mathbf{k})\hat{R}^{-1}$ is a Bloch state operator at $R\mathbf{k}$ with the same energy. Therefore, in general,

$$\hat{R}\gamma_n(\mathbf{k})\hat{R}^{-1} = \sum_{m\in\text{occ}} [\mathcal{B}_R(\mathbf{k})]_{mn}\gamma_m(R\mathbf{k}), \tag{11}$$

where $m \in$ occ. Considering degeneracies, $[\mathcal{B}_R(\mathbf{k})]_{mn}$ is *not* proportional to δ_{mn}. The N_{occ}-by-N_{occ} matrix $\mathcal{B}_R(\mathbf{k})$ is called the sewing matrix associated with PGS operator R, and we will keep using curly letters to represent matrices in the space of occupied bands. Defining $|\psi_n(\mathbf{k})\rangle = \gamma_n^\dagger(\mathbf{k})|0\rangle$, where $|0\rangle$ is the vacuum state with no fermion, we can also put the sewing matrix definition in the form

$$[\mathcal{B}_R(\mathbf{k})]_{mn} = \langle\psi_m(R\mathbf{k})|\hat{R}|\psi_n(\mathbf{k})\rangle, \tag{12}$$

for $m,n \in$ occ. (Throughout the paper, when it is a greek letter inside $|\rangle/\langle|$, the symbol denotes a column/row vector in the single-particle Hilbert space.)

An alternative and useful expression of the sewing matrix can be found by noticing that each Bloch state $|\psi_n(\mathbf{k})\rangle$ is the direct product of a plane wave $e^{i\mathbf{k}\cdot\mathbf{r}}$ and an orbital part $|u_n(\mathbf{k})\rangle$, and noticing that the rotation operator $\hat{R}$ acts on the two parts separately sending $e^{i\mathbf{k}\cdot\mathbf{r}}$ to $e^{iR\mathbf{k}\cdot\mathbf{r}}$ and $|u_n(\mathbf{k})\rangle$ to $\tilde{R}|u_n\rangle$:

$$[\mathcal{B}_R(\mathbf{k})]_{mn} = \langle u_m(R\mathbf{k})|\tilde{R}|u_n(\mathbf{k})\rangle, \tag{13}$$

where $\tilde{R}$ and all capital letters with a tilde are matrices in the orbital space and when a roman letter appears in $|\rangle/\langle|$, the symbol denotes a column/row vector in the orbital space.

For a given PGS operator R, there are points in BZ at which $\mathbf{k}_{\text{inv}} = R\mathbf{k}_{\text{inv}}$. These points are called high-symmetry points, or points of symmetry. At $\mathbf{k}_{\text{inv}}$, from Eq. (8), we have

$$[\hat{R}, \hat{h}(\mathbf{k}_{\text{inv}})] = 0. \tag{14}$$

Therefore we can find a common set of eigenstates of both $\hat{R}$ and $\hat{h}(\mathbf{k}_{\text{inv}})$. In that basis, the sewing matrix is diagonal:

$$[\mathcal{B}_R(\mathbf{k}_{\text{inv}})]_{mn} = R_m(\mathbf{k})\delta_{mn}, \tag{15}$$

where R_m is the eigenvalue of $\hat{R}$ on the mth band. The determinant of the sewing matrix at $\mathbf{k}_{\text{inv}}$ can then be calculated as, using Eq. (15),

$$\det[\mathcal{B}_R(\mathbf{k}_{\text{inv}})] = \prod_{n\in\text{occ}} R_n(\mathbf{k}_{\text{inv}}). \tag{16}$$

Since the determinant is independent of the choice of basis, $\det[\mathcal{B}_R(\mathbf{k}_{\text{inv}})]$ is a gauge invariant quantity.

C. Monodromy

Path-ordered loop integrals and line integrals of exponentiated Berry connection are extensively used in Sec. III A. Here, we briefly develop basic properties of these integrals. Alternative formulas can be found in Ref. 36.

A path-ordered loop integral of Berry connection describes a unitary evolution of the linear subspace spanned by the N_{occ} eigenstates of $\tilde{H}(\mathbf{k})$ around a closed circuit in the BZ. Mathematically, it is expressed in terms of the non-Abelian Berry connection,

$$\mathcal{W}_L = P\exp[i\oint_L \mathcal{A}(\mathbf{k})\cdot d\mathbf{k}], \tag{17}$$

where L means a closed loop and P means "path ordered." Here, we point out that in 2D, the determinant of this integral

$$\begin{aligned}\det(\mathcal{W}_L) &= \det\left\{P\exp\left[i\oint_L \mathcal{A}(\mathbf{k})\cdot d\mathbf{k}\right]\right\}\\ &= \det\left\{\exp\left[i\oint_L \mathcal{A}(\mathbf{k})\cdot d\mathbf{k}\right]\right\}\\ &= \exp\left\{i\,\text{Tr}\left[\oint_L \mathcal{A}(\mathbf{k})\cdot d\mathbf{k}\right]\right\}\\ &= \exp(i\phi_B),\end{aligned} \tag{18}$$

where ϕ_B is the Berry phase associated with the loop.

In Sec. III A, we will calculate the determinants of loop integrals that encircle a portion of BZ. To calculate them, it is convenient to define the Wilson line between the occupied-subspaces at $\mathbf{k}_1$ and $\mathbf{k}_2$, obtained by exponentiating the Berry connection:

$$\mathcal{U}_{\mathbf{k}_1\mathbf{k}_2} = P\exp\left[i\int_{\mathbf{k}_2}^{\mathbf{k}_1} \mathcal{A}(\mathbf{k})d\mathbf{k}\right]. \tag{19}$$

In a finite system with discrete $\mathbf{k}$, we have, equivalently,

$$\begin{aligned}&(\mathcal{U}_{\mathbf{k}_1\mathbf{k}_2})_{mn}\\ &= \sum_{a,b\ldots}\langle u_m(\mathbf{k}_1)|u_a(\mathbf{k}_1')\rangle\langle u_a(\mathbf{k}_1')|u_b(\mathbf{k}_2')\rangle\langle u_b(\mathbf{k}_2')|\ldots|u_n(\mathbf{k}_2)\rangle,\end{aligned} \tag{20}$$

where $\mathbf{k}_1', \mathbf{k}_2', \ldots$ form a path connecting $\mathbf{k}_1$ and $\mathbf{k}_2$.

This connection is by definition an $N_{\text{occ}} \times N_{\text{occ}}$ matrix. We can also define an orbital space operator $\tilde{U}_{\mathbf{k}_1\mathbf{k}_2}$ associated with this matrix:

$$\begin{aligned}\tilde{U}_{\mathbf{k}_1\mathbf{k}_2} &= \sum_{i,j\in\text{occ}} \left(\mathcal{U}_{\mathbf{k}_1\mathbf{k}_2}\right)_{ij}|u_i(\mathbf{k}_1)\rangle\langle u_j(\mathbf{k}_2)|\\ &= P\exp\left(i\int_{\mathbf{k}_2}^{\mathbf{k}_1}\tilde{P}_\mathbf{k}\partial\tilde{P}_\mathbf{k}\cdot d\mathbf{k}\right),\end{aligned} \tag{21}$$

where $\tilde{P}_\mathbf{k} = \sum_{i\in\text{occ}}|u_i(\mathbf{k})\rangle\langle u_i(\mathbf{k})|$ is the projector onto the occupied subspace at $\mathbf{k}$. In a finite size system, alternatively, one has

$$\tilde{U}_{\mathbf{k}_1\mathbf{k}_2} = \tilde{P}_{\mathbf{k}_1}\left(\prod_{j=1,2,\ldots}\tilde{P}_{\mathbf{k}_j'}\right)\tilde{P}_{\mathbf{k}_2}. \tag{22}$$

The advantage of using $\tilde{U}_{\mathbf{k}_1\mathbf{k}_2}$ is its gauge invariance as $\tilde{P}_{\mathbf{k}}$ only depends on the Hamiltonian. If the Hamiltonian has a symmetry R, it can be proven that

$$\tilde{R}\tilde{U}_{\mathbf{k}_1\mathbf{k}_2}\tilde{R}^{-1} = \tilde{U}_{R\mathbf{k}_1 R\mathbf{k}_2}, \tag{23}$$

although no simple relation exists for their corresponding matrices in the occupied band space $\mathcal{U}_{\mathbf{k}_1\mathbf{k}_2}$ and $\mathcal{U}_{R\mathbf{k}_1 R\mathbf{k}_2}$. This property will be extensively used in the monodromy proof provided in Sec. III A.

III. TWO-DIMENSIONAL INSULATORS WITH CYCLIC POINT GROUP SYMMETRIES

There are in total ten point groups in 2D. One is the trivial group containing only the identity, and among the nontrivial nine PGS, there are four cyclic PGS denoted by $C_{n=2,3,4,6}$. The symmetry group C_n is generated by an n-fold rotation about the z axis that is out of plane. In this section, we will study C_n-invariant insulators in two dimensions.

A. Chern number in terms of rotation eigenvalues at high-symmetry points

In the following, we endeavor to prove in a C_n-invariant insulator, the Chern number modulo n is given by C_m eigenvalues of all occupied bands at each C_m-invariant $\mathbf{k}$ point for each m dividing n. The case of $n = 2$ has been studied in Ref. 32 and the result is

$$(-1)^C = \prod_{i\in\text{occ.}} \zeta_i(\Gamma)\zeta_i(X)\zeta_i(Y)\zeta_i(M), \tag{24}$$

where $\zeta_i(\mathbf{k} = \Gamma, X, Y, M)$ is the eigenvalue of the operator $\hat{C}_2$ at C_2-invariant $\mathbf{k}$ point on the ith band. This equation shows that the parity (even or odd) of the Chern number can be determined by knowing the inversion eigenvalues at four high-symmetry points.

Now we move beyond the simple and already discussed case of C_2 symmetric systems to calculate the Chern number in C_n-invariant insulators for $n = 3,4,6$. We will calculate the Chern number by relating it to the determinant of a special closed loop integral of exponentiated Berry connection defined in BZ. In the main text, the detailed calculation is only shown for C_4-invariant insulators; for $C_{3,6}$-invariant insulators, the main conclusions are stated here, while details are provided in Appendix B.

For $n = 4$, the loop is chosen as $\lambda = \Gamma XMY\Gamma$ shown in Fig. 1(b), and the determinant of the path-ordered loop integral becomes

$$\det\left\{P\exp\left[\oint_\lambda \mathcal{A}(\mathbf{k})\cdot d\mathbf{k}\right]\right\} = e^{i\pi C/2}. \tag{25}$$

To prove this, we note that due to C_4, we have the following symmetry in the field strength:

$$\text{Tr}[\mathcal{F}_{xy}(k_x,k_y)] = \text{Tr}[\mathcal{F}_{xy}(-k_y,k_x)] \tag{26}$$

(for a proof see Appendix E) and hence the integral of Berry phase inside λ is one-fourth of the Berry phase in the whole BZ ($2\pi C$). On the other hand, the loop integral is given by the connection matrices defined in Sec. II C:

$$\mathcal{W}_\lambda = \mathcal{U}_{\Gamma X}\mathcal{U}_{XM}\mathcal{U}_{MY}\mathcal{U}_{Y\Gamma}. \tag{27}$$

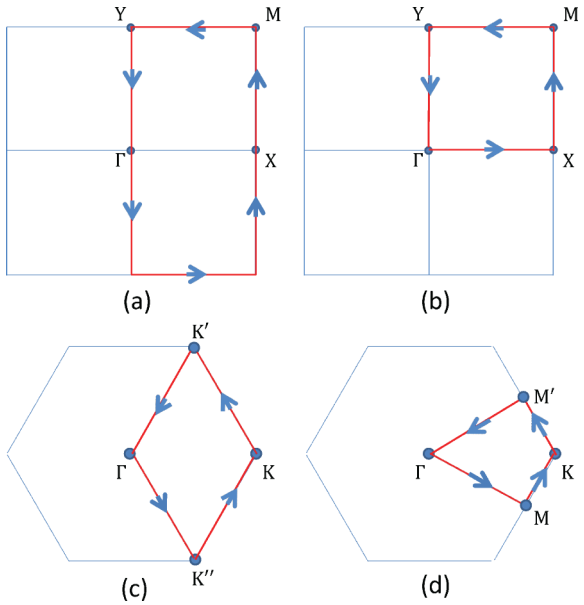


FIG. 1. (Color online) Schematic of the loop integrals used in the monodromy proof of the relationship between the Chern number and the eigenvalues at high-symmetry points within the Brillouin zone in C_n-invariant topological insulators with $n = 2,4,3,6$ in (a), (b),(c), and (d), respectively.

With C_4 symmetry at hand and utilizing the periodicity of the BZ, we notice that $\tilde{C}_4\tilde{U}_{\Gamma Y}\tilde{C}_4^{-1} = \tilde{U}_{\Gamma X}$ and $\tilde{C}_4^{-1}\tilde{U}_{YM}\tilde{C}_4 = \tilde{U}_{MX}$. We may further simplify the determinant as (see Appendix A for more additional details)

$$\begin{aligned}\det(\mathcal{W}_\lambda) &= \det\left[\mathcal{B}_{C_4}(\Gamma)\mathcal{U}_{\Gamma Y}\mathcal{B}_{C_2}(Y)^{-1}\mathcal{U}_{YM}\mathcal{B}_{C_4}(M)\mathcal{U}_{MY}\mathcal{U}_{Y\Gamma}\right]\\ &= \det\left[\mathcal{B}_{C_4}(\Gamma)\mathcal{B}_{C_2}^{-1}(Y)\mathcal{B}_{C_4}(M)\right]\det(\mathcal{U}_{\Gamma Y}\mathcal{U}_{YM}\mathcal{U}_{MY}\mathcal{U}_{Y\Gamma})\\ &= \det\left[\mathcal{B}_{C_4}(\Gamma)\mathcal{B}_{C_2}^{-1}(Y)\mathcal{B}_{C_4}(M)\right],\end{aligned} \tag{28}$$

where we have used $\mathcal{U}_{YM} = \mathcal{U}_{MY}^{-1}$. From Eqs. (25), (29), and (16), we obtain

$$i^C = \prod_{n\in\text{occ.}} \xi_n(\Gamma)\xi_n(M)\zeta_n^{-1}(Y), \tag{29}$$

where $\xi_i(\mathbf{k})$ is the eigenvalue of $\hat{C}_4$ at the C_4-invariant $\mathbf{k}$ point on the ith band. Since $\hat{C}_2^2 = (-1)^F$, we have $\zeta^2(\mathbf{k} = X,Y) = (-1)^F$ or

$$\zeta^{-1}(Y) = (-1)^F\zeta(Y). \tag{30}$$

Substituting Eq. (30) into Eq. (29), we obtain

$$i^C = \prod_{i\in\text{occ.}} (-1)^F\xi_i(\Gamma)\xi_i(M)\zeta_i(Y). \tag{31}$$

Equation (31) tells us that given the eigenvalues of $\hat{C}_4$ at Γ, M and those of $\hat{C}_2$ at Y, one can determine the Chern number up to a multiple of four. It may be disconcerting that in Eq. (31), we only include the C_2 eigenvalues at Y but not at X, but in fact they are identical: in systems with C_4 symmetry, $\zeta_i(0,\pi) = \zeta_i(\pi,0)$ as the two points are related by C_4 rotation.

For $n = 3$ and 6, the proof takes very similar steps which we leave to Appendix B, and only differs in that one chooses the loops as shown in Figs. 1(c) and 1(d), respectively. We

simply quote the salient results here:

$$e^{i2\pi C/3} = \prod_{i\in\text{occ.}} (-1)^F \theta_i(\Gamma)\theta_i(K)\theta_i(K'), \tag{32}$$

$$e^{i\pi C/3} = \prod_{i\in\text{occ.}} (-1)^F \eta_i(\Gamma)\theta_i(K)\zeta_i(M), \tag{33}$$

where $\theta_i(\mathbf{k})$ and $\eta_i(\mathbf{k})$ represent the eigenvalues of $\hat{C}_3$ and $\hat{C}_6$ at C_3- and C_6-invariant $\mathbf{k}$ points, respectively.

B. Chern number in terms of the C_n eigenvalue of the Slater determinant

We have shown how the Chern number is related to symmetry eigenvalues of the single-particle states at high-symmetry points. Now we will see that another connection between the Chern number and C_n-invariance presents itself as one considers the C_n eigenvalue of the *many-body* ground state (under the assumption that this is nondegenerate), or the Slater determinant state of a C_n-invariant insulator:

$$\exp\left(iC\frac{2\pi}{n}\right) = f_n(N)\rho_n, \tag{34}$$

where $f_n(N)$ is either $+1$ or -1 depending on the total number of sites and ρ_n is the eigenvalue of $\hat{C}_n$ of the Slater determinant state $|\Phi_0\rangle$, i.e., $\hat{C}_n|\Phi_0\rangle = \rho_n|\Phi_0\rangle$. Equation (34) can be proved by expressing ρ_n in terms of the eigenvalues of the single-particle states at high-symmetry points and then using Eqs. (24), (32), (31), and (33) to relate ρ_n to the Chern number for $n = 2,3,4,6$.

We begin by looking at the case of C_2-invariant insulators. The Slater determinant of the ground state is given by

$$|\Phi_0\rangle = \prod_{\mathbf{k}\in\text{BZ}} \prod_{i\in\text{occ.}} \gamma_i^\dagger(\mathbf{k})|0\rangle. \tag{35}$$

We can pair $\mathbf{k}$ and $-\mathbf{k}$ and this results in only four $\mathbf{k}$'s that cannot be paired as they are inversion invariant. So the Slater determinant can be written as

$$|\Phi_0\rangle = \prod_{i\in\text{occ.}} \gamma_i^\dagger(\Gamma)\gamma_i^\dagger(Y)\gamma_i^\dagger(X)\gamma_i^\dagger(M) \times \prod_{\mathbf{k}\in BZ/2} (\gamma_i^\dagger(\mathbf{k})\gamma_i^\dagger(-\mathbf{k}))|0\rangle. \tag{36}$$

Note that in writing down the above equation, and throughout the rest of the section, we have implicitly assumed that all high-symmetry points exist in the finite system, and for a discussion of all other cases, see Appendix C. Now consider the action of $\hat{C}_2$ on this state:

$$\begin{aligned}\hat{C}_2|\Phi_0\rangle &= \prod_{i\in\text{occ}} [\hat{C}_2\gamma_i^\dagger(\Gamma)\hat{C}_2^{-1}][\hat{C}_2\gamma_i^\dagger(Y)\hat{C}_2^{-1}][\hat{C}_2\gamma_i^\dagger(X)\hat{C}_2^{-1}][\hat{C}_2\gamma_i^\dagger(M)\hat{C}_2^{-1}] \prod_{\mathbf{k}\in\text{BZ}/2} [\hat{C}_2\gamma_i^\dagger(\mathbf{k})\hat{C}_2^{-1}\hat{C}_2\gamma_i^\dagger(-\mathbf{k})\hat{C}_2^{-1}]|\Phi_0\rangle \\ &= (-1)^{N_{\text{occ}}(N-4)/2} \det\left[\mathcal{B}_{C_2}(\Gamma)\right]\det\left[\mathcal{B}_{C_2}(X)\right]\det\left[\mathcal{B}_{C_2}(Y)\right]\det\left[\mathcal{B}_{C_2}(M)\right] \prod_{\mathbf{k}\in\text{BZ}/2} \det\left[\mathcal{B}_{C_2}(\mathbf{k})\mathcal{B}_{C_2}(-\mathbf{k})\right]|\Phi_0\rangle.\end{aligned} \tag{37}$$

Using the sewing matrix property to see that $\mathcal{B}_{C_2}(\mathbf{k}) = (-1)^F\mathcal{B}_{C_2}^{-1}(-\mathbf{k})$, one obtains from Eq. (37),

$$\hat{C}_2|\Phi_0\rangle = (-1)^{\frac{(F-1)N_{\text{occ}}(N-4)}{2}} \prod_{i\in\text{occ.}} \zeta_i(\Gamma)\zeta_i(X)\zeta_i(Y)\zeta_i(M)|\Phi_0\rangle. \tag{38}$$

Combining Eqs. (38) and (24), we have

$$(-1)^C = (-1)^{(F-1)N_{\text{occ}}N/2}\rho_2 \tag{39}$$

for C_2-invariant insulators.

The case with $n = 4$ can be similarly studied. Here, four generic $\mathbf{k}$'s can be grouped with the exception of the Γ and M points, which do not pair with any other $\mathbf{k}$ as they are invariant under C_4. Additionally, X and Y pair between themselves to make a group of two. The Slater determinant is then given by

$$\begin{aligned}|\Phi_0\rangle &= \prod_{i\in\text{occ}} \left\{\gamma_i^\dagger(\Gamma)\gamma_i^\dagger(M)[\gamma_i^\dagger(X)\gamma_i^\dagger(Y)] \prod_{\mathbf{k}\in\text{BZ}/4,\mathbf{k}\neq\mathbf{k}_{\text{inv}}} [\gamma_i^\dagger(k_x,k_y)\gamma_i^\dagger(-k_y,k_x)\gamma_i^\dagger(-k_x,-k_y)\gamma_i^\dagger(k_y,-k_x)]\right\}|0\rangle \\ &= (-1)^{N_{\text{occ}}N/4}\det\left[\mathcal{B}_{C_4}(\Gamma)\right]\det\left[\mathcal{B}_{C_4}(M)\right]\det\left[\mathcal{B}_{C_4}(X)\mathcal{B}_{C_4}(Y)\right] \\ &\quad\times \prod_{\mathbf{k}\in\text{BZ}/4,\mathbf{k}\neq\mathbf{k}_{\text{inv}}} \det\left[\mathcal{B}_{C_4}(k_x,k_y)\mathcal{B}_{C_4}(-k_y,k_x)\mathcal{B}_{C_4}(-k_x,-k_y)\mathcal{B}_{C_4}(k_y,-k_x)\right]|\Phi_0\rangle.\end{aligned} \tag{40}$$

Since C_4 is a fourfold rotation, two consecutive C_4's equal a twofold rotation, and that four consecutive C_4's equal a complete rotation. In terms of sewing matrices, these simple facts are represented by

$$\begin{aligned}\mathcal{B}_{C_4}(X)\mathcal{B}_{C_4}(Y) &= \mathcal{B}_{C_2}(X), \\ \mathcal{B}(\mathbf{k})\mathcal{B}(C_4\mathbf{k})\mathcal{B}(C_4^2\mathbf{k})\mathcal{B}(C_4^3\mathbf{k}) &= (-1)^F.\end{aligned} \tag{41}$$

By substituting these relations into Eq. (40), we obtain

$$\hat{C}_4|\Phi_0\rangle = (-1)^{N_{\text{occ}}[(F-1)N/4+F]} \prod_{i\in\text{occ}} \xi_i(\Gamma)\xi_i(M)\zeta_i(X)|\Phi_0\rangle. \tag{42}$$

Combining Eqs. (42) and (31), we have

$$i^C = (-1)^{(F-1)N_{\text{occ}}N/4}\rho_4. \tag{43}$$

Finally, we discuss systems possessing C_3 symmetry and C_6 in a straightforward fashion. Here, with the exception of the three $\mathbf{k}$'s that are invariant under C_3: Γ, K, and K', whose corresponding Bloch state operators $\gamma_i(\mathbf{k}_{\rm inv})$ cannot be grouped in threes in the Slater determinant for each band, all other $\gamma_i(\mathbf{k})$'s (i.e., at other $\mathbf{k}$'s) can be grouped in threes. Following the same procedure, one finds

$$\hat{C}_3|\Phi_0\rangle = \prod_{i\in\text{occ}} \theta_i(\Gamma)\theta_i(K)\theta_i(K') \times \prod_{\mathbf{k}\in \text{BZ}/3, \mathbf{k}\neq\mathbf{k}_{\rm inv}} \det\left[\mathcal{B}(\mathbf{k})\mathcal{B}(C_3\mathbf{k})\mathcal{B}\left(C_3^2\mathbf{k}\right)\right]|\Phi_0\rangle. \quad (44)$$

Since $\det[B(\mathbf{k})B(C_3\mathbf{k})B(C_3^2\mathbf{k})] = (-1)^F$ because three C_3's equal a complete rotation, we have

$$\hat{C}_3|\Phi_0\rangle = (-1)^{FN_{\rm occ}(N-3)/3} \prod_{i\in\text{occ}} \theta_i(\Gamma)\theta_i(K)\theta_i(K')|\Phi_0\rangle. \quad (45)$$

Therefore the Chern number can be expressed in terms of ρ_3 as

$$\exp\left(iC\frac{2\pi}{3}\right) = (-1)^{FN_{\rm occ}N/3}\rho_3. \quad (46)$$

For C_6 invariant insulators, similar steps (not shown here) lead to

$$\exp\left(iC\frac{\pi}{3}\right) = (-1)^{FN_{\rm occ}N/6}\rho_6. \quad (47)$$

Up to this point we have proved Eq. (34) for all C_n-invariant insulators. Physically, it shows that the Chern number modulo n in a C_n invariant insulator is exactly the total angular momentum of the ground state. Although the Chern number was originally defined in terms of the Berry connection of single-particle states, one can generalize its definition to an interacting system using flux insertion, also known as the distorted periodic boundary conditions, if the ground-state is nondegenerate. It is then straightforward to see that in a weakly interacting system, the relation between the Chern number and the total angular momentum of ground state still holds because both numbers are quantized and therefore cannot change infinitesimally as interaction is adiabatically turned on. This relation largely simplifies the calculation of Chern number in a weakly interacting system, because only ground-state information with normal boundary condition is needed to obtain the total angular momentum, or the C_n eigenvalue.

IV. TWO-DIMENSIONAL INSULATORS WITH DIHEDRAL POINT GROUPS

Out of 9 nontrivial PGS in 2D, five are called diheral PGS, denoted by $D_{n=1,2,3,4,6}$. The structure of the diheral group is simple: $D_n = C_n \cup (C_2' * C_n)$, where C_2' is a twofold rotation about some in-plane axis (referred to as x axis in later text). For later discussion, we define the basis vectors in the real space and reciprocal space in four out of five 2D Braivis lattices in Fig. 2: rectangular, centered rectangular, square, and triangular lattices. The parallelogram lattice is excluded from the discussion as it cannot be D_n invariant.

In 2D, D_n group is identical to C_{nv} group for spinless particles, where C_{nv} is generated by C_n and a mirror plane of

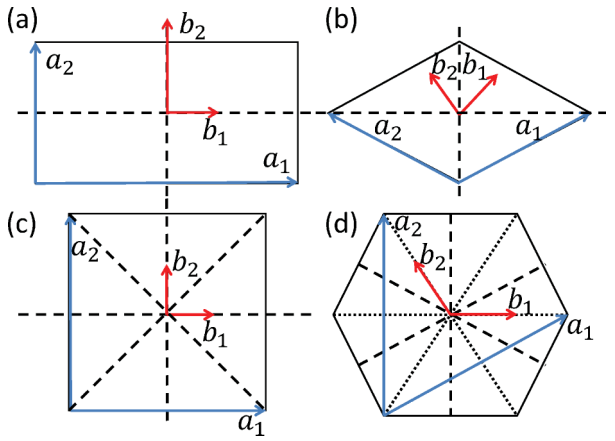


FIG. 2. (Color online) Primitive cells of four 2D Braivis lattices: (a) rectangle, (b) centered-rectangle, (c) square, and (d) triangle. The basis vectors of the real lattice $\mathbf{a}_{1,2}$ are plotted as blue arrows and the basis vectors of the reciprocal lattice $\mathbf{b}_{1,2}$ are plotted as red arrows. All possible C_2' axes are plotted as dashed lines in (a)–(c). In (d), dashed lines and dotted lines represent two sets of C_2' axes. D_3 PGS includes either one of the two sets and D_6 PGS contains both sets.

xz, M_{xz}. This is because both C_2' and M_{xz} will send (x,y) to $(x,-y)$. For spin-1/2 particles, the C_2' acts as σ_z in the spin space, while M_{xz} acts as σ_y in the spin space. Therefore, in principle, a C_{nv}-symmetric 2D system is *not* a D_n-symmetric system. However, throughout the section below, they are completely equivalent, because we only need a symmetry that sends a state at (k_x,k_y) to one at $(k_x,-k_y)$ of the same energy and both C_2' and M_{xz} have this property. Therefore all conclusions obtained here apply to C_{nv}-symmetric insulators without any adaptation.

A. Vanishing Chern number

A dihedral PGS has a strong constraint on the Hall conductance of a 2D insulator:

$$\sigma_{xy} = 0. \quad (48)$$

Since in a noninteracting insulator the Hall conductance is proportional to the Chern number, Eq. (48) implies that the Chern number of an insulator with any dihedral PGS must be trivial. A heuristic understanding of Eq. (48) is that since σ_{xy} changes sign under C_2', if the system is C_2' invariant, σ_{xy} can only be zero. This simple argument can be put in a rigorous form presented in Appendix D. An alternative proof of the vanishing Chern number is by using the general transform property of field strength $\mathcal{F}_{xy}$ Eq. (83) proved in Appendix E, and substituting $R = C_2'$ to obtain

$$\mathcal{F}_{xy}(k_x,-k_y) = -\mathcal{B}_{C_2'}(k_x,k_y)\mathcal{F}_{xy}(k_x,k_y)\mathcal{B}^\dagger_{C_2'}(k_x,k_y). \quad (49)$$

Substituting Eq. (49) into Eq. (1), we find

$$\begin{aligned} C &= \frac{1}{2\pi}\int_{-\pi}^{\pi} dk_x \left\{\int_{-\pi}^{0} \text{Tr}[\mathcal{F}_{xy}(\mathbf{k})]dk_y + \int_{0}^{\pi} \text{Tr}[\mathcal{F}_{xy}(\mathbf{k})dk_y]\right\} \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} dk_x \int_{0}^{\pi} \text{Tr}[\mathcal{F}_{xy}(k_x,k_y) + \mathcal{F}_{xy}(k_x,-k_y)]dk_y \\ &= 0. \end{aligned} \quad (50)$$

Although Eqs. (48) and (50) are equivalent to each other in a noninteracting insulator, in an interacting insulator with diheral PGS, Eq. (50) loses its meaning due to the absence of Bloch states, but Eq. (48) still holds.

B. Quantization of the electric polarization

As the Chern number always vanishes in these insulators, we need some other bulk topological invariant to identify nontrivial D_n-invariant 2D insulators. When Chern number vanishes, one can always find a continuous gauge, or a choice of continuous Bloch wave functions on the whole BZ with periodic boundary condition. With this gauge choice it can be proved that the electric polarization, or the center of charge, is unambiguously defined within a unit cell, and its position vector is given by

$$\mathbf{P} = p_1\mathbf{a}_1 + p_2\mathbf{a}_2, \tag{51}$$

where $\mathbf{a}_{1,2}$ are the unit cell basis vectors of the lattice and $p_{1,2}$ are in general within the range $[0,1)$., given by the integral of the Berry connection:[37]

$$p_i = \frac{1}{2\pi}\int_0^1 dk_1 \int_0^1 dk_2 \mathrm{Tr}[\mathcal{A}_i(k_1\mathbf{b}_1 + k_2\mathbf{b}_2)], \tag{52}$$

where k_i is the component of $\mathbf{k}$ in its linear expansion in reciprocal lattice vectors $\mathbf{b}_{1,2}$. Here we briefly discuss why the vanishing of Chern number is necessary for the definition of polarization, taking $i = 1$, for example. First notice that $\int dk_1 \mathrm{Tr}[\mathcal{A}_1(k_1,k_2)] = P_1(k_2)$ is the 1D polarization at fixed k_2. If the Chern number is nonzero, this number changes by exactly C from $k_2 = 0$ to $k_2 = 1$. Therefore the integral in Eq. (52) depends on the integration range of k_2. For example, the integral takes different values for integrating in $[\delta, 1+\delta)$ and in $[0,1)$. Since no physical quantity should depend on the choice of BZ, the polarization in this case is meaningless.

Before presenting the formal results of quantized electric polarization in D_n-invariant insulators, it is helpful to establish an intuitive understanding. First, we remember that the electric polarization is quantized to 0 and $1/2$ (in unit eL where L is the length of the system) in a 1D insulator with inversion symmetry. This result can be easily understood in a heuristic way: suppose the system has polarization p, but due to inversion, the polarization is also $-p$. Then since p is only well defined up to an integer, the only possible values of p are $p = 0$ and $p = 1/2$. Now given a D_4-invariant system with polarization (p_1, p_2), then from C_4 invariance it must be equivalent to $(-p_2, p_1)$, and since both p_1 and p_2 are defined up to an integer, we have equations $p_1 = -p_2 + \text{integer}$ and $p_2 = p_1 + \text{integer}$, the only solutions to which are $p_1 = p_2 = 0$ and $p_1 = p_2 = 1/2$. One is reminded, however, that although we only used C_4 to prove the quantization of $p_{1,2}$, we implicitly assumed that the Chern number is zero, without which the polarization is undefined. (This important fact is obscured in this heuristic picture.) Following the same approach, one can prove that for $D_{3,6}$-invariant insulators, (p_1, p_2) is also quantized and the quantized values can be similarly written down. Despite being physically clear, this simple argument does not serve as a proof of the our statement, and, furthermore, it does not give the actual value of (p_1, p_2) for a given band structure. In what follows, we prove the quantization of electric polarization in D_n-invariant insulators analytically and express the quantized polarization in terms of C_n eigenvalues at points of symmetry.

Now we prove that C_n PGS, a subgroup of D_n PGS, quantizes $p_{1,2}$. Using sewing matrix $\mathcal{B}_{C_n}$, we have

$$\begin{aligned} p_i &= \frac{i}{2\pi}\int dk_1 dk_2 \mathrm{Tr}\langle u(\mathbf{k})|\tilde{C}_n^\dagger \frac{d}{dk_i}\tilde{C}_n|u(\mathbf{k})\rangle \\ &= \frac{i}{2\pi}\int dk_1 dk_2 \mathrm{Tr}\langle u(C_n\mathbf{k})|\mathcal{B}_{C_n}^\dagger(\mathbf{k})\frac{d}{dk_i}\mathcal{B}_{C_n}(\mathbf{k})|u(C_n\mathbf{k})\rangle \\ &= \frac{i}{2\pi}\int dk_1 dk_2 \mathrm{Tr}\langle u(C_n\mathbf{k})|\frac{d}{dk_i}|u(C_n\mathbf{k})\rangle \\ &\quad + i\int \mathrm{Tr}\left[\mathcal{B}_{C_n}(\mathbf{k})^\dagger \frac{d}{dk_i}\mathcal{B}_{C_n}(\mathbf{k})\right]dk_1 dk_2. \end{aligned} \tag{53}$$

Using the unitarity of $\mathcal{B}_{C_n}(\mathbf{k})$, the integrand in second term of the last line can be rewritten as

$$\mathrm{Tr}\left[\mathcal{B}_{C_n}(\mathbf{k})^\dagger \frac{d}{dk_i}\mathcal{B}_{C_n}(\mathbf{k})\right] = \frac{d}{dk_i}\ln\left\{\det\left[\mathcal{B}_{C_n}(\mathbf{k})\right]\right\}. \tag{54}$$

Substituting Eq. (54) to the second integral of last line of Eq. (53), we find (taking $i = 1$, for example, while the same proceeds for $i = 2$)

$$\begin{aligned} &\frac{i}{2\pi}\int dk_1 dk_2 \mathrm{Tr}\left[\mathcal{B}_{C_n}(k_1,k_2)^\dagger \frac{d}{dk_1}\mathcal{B}_{C_n}(k_1,k_2)\right] \\ &\quad = \frac{i}{2\pi}\int dk_2\left(\int dk_1 \frac{d\ln\left\{\det\left[\mathcal{B}_{C_n}(k_1,k_2)\right]\right\}}{dk_1}\right). \end{aligned} \tag{55}$$

The integral over k_1 will give $2q_1\pi i$, where q_1 is the winding number of $\det(\mathcal{B}_{C_n})$, which is a pure phase, at a fixed k_2. However, we have chosen a smooth gauge so $q_1(k_2)$ must be a smooth function of k_2, which, in the case of a discrete function, is a constant. That is to say, the winding at each k_2 must be the same. Therefore we have

$$\begin{aligned} &\frac{i}{2\pi}\int dk_1 dk_2 \mathrm{Tr}\left[\mathcal{B}_{C_n}(k_1,k_2)^\dagger \frac{d}{dk_1}\mathcal{B}_{C_n}(k_1,k_2)\right] \\ &\quad = \int dk_2 q_1(k_2) \qquad (56) \\ &\quad = q_1 \in Z. \qquad (57) \end{aligned}$$

Using Eq. (56) in the last line of Eq. (53), we have

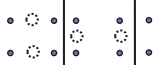
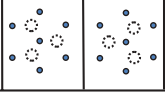
$$p_i = \frac{i}{2\pi}\int k_1 k_2 \mathrm{Tr}\langle u(C_n\mathbf{k})|\frac{d}{dk_i}|u(C_n\mathbf{k})\rangle + q_i(C_n). \tag{58}$$

The first term of the right-hand side of Eq. (58) may be further simplified using

$$\begin{aligned} \langle u(C_n\mathbf{k})|\frac{d}{dk_i}|u(C_n\mathbf{k})\rangle &= \frac{\langle u(C_n\mathbf{k})|u(C_n\mathbf{k} + dk_i C_n\mathbf{b_i})\rangle - 1}{dk_i} \\ &= R^{(n)}_{ij}\langle u(\mathbf{k}')|\frac{d}{dk'_j}|u(\mathbf{k}')\rangle|_{\mathbf{k}'=C_n\mathbf{k}}, \end{aligned} \tag{59}$$

where $R^{(n)}$ is the 2×2 matrix describing the rotation of the basis vectors $\mathbf{b}_{1,2}$ under C_n, summarized in the second row of Table III. Inserting Eq. (59) into Eq. (58) and after some

TABLE III. Quantized values of electric polarization (p_1, p_2) in $D_{n=2,3,4,6}$-invariant 2D insulators. From the first row: the value of n in D_n, the transform matrix $R^{(n)}$ of n-fold rotation in the basis of $\mathbf{b}_{1,2}$, the unit cell in the Bravais lattice with all C_2' axes, symmetry constraints on the values of $p_{1,2}$ by C_n, additional constraints by C_2', all nontrivial (p_1, p_2) pairs, the visualization of the charge center (large dotted circle) in the lattice defined by solid dots.

$n = 2$		$n = 3$		$n = 4$	$n = 6$
$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$		$\begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix}$		$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 \\ -1 & 0 \end{pmatrix}$
					
$2p_1 = q_1$ $2p_2 = q_2$		$p_1 - p_2 = q_1$ $p_1 + 2p_2 = q_2$		$2p_1 = 2p_2 = q_1$	$p_1, p_2 \in Z$
	$p_1 - p_2 \in Z$		$p_2 \in Z$		
$(\frac{1}{2}, 0)$ $(0, \frac{1}{2})$ $(\frac{1}{2}, \frac{1}{2})$	$(\frac{1}{2}, \frac{1}{2})$	$(\frac{2}{3}, \frac{2}{3})$ $(\frac{1}{3}, \frac{1}{3})$		$(\frac{1}{2}, \frac{1}{2})$	
					

rearrangement, we obtain

$$p_i - \sum_j R_{ij}^{(n)} p_j = q_i(C_n) \in Z. \tag{60}$$

Equation (60) is the general form of symmetry constraints by C_n invariance on the electric polarization.

In addition to the constraints by C_n symmetry, C_2' symmetry also puts constraints on (p_1, p_2). These constraints are derived in a way very similar to the way sketched in Eqs. (53)–(58). The result is given in the same form of Eq. (60):

$$p_i - \sum_j R_{ij}^{'(2)} p_j = q_i(C_n) \in Z. \tag{61}$$

Where $R^{'(2)}$ is the transformation matrix of the basis $\mathbf{b}_{1,2}$ under the twofold rotation C_2' (also listed in Table III). One can see in many cases, this additional symmetry does not give any additional constraints/quantization of $p_{1,2}$, but there are a few important exceptions. For $n = 1$, i.e., when there is no rotation symmetry about z axis, the C_2' symmetry gives quantization to the polarization perpendicular to the rotation axis (defined as x axis). This is because for this system, at each k_x, $H(k_x, k_y)$ is a 1D inversion symmetric insulator whose polarization is quantized, and due to continuity of the gauge, the polarization is the same for all k_x. Therefore the total polarization is quantized. For D_2 insulators, if the C_2' axis coincides with the bisect of $\mathbf{a}_1$ and $\mathbf{a}_2$, i.e., in the case of centered-rectangle lattice, the C_2' rotation symmetry gives $p_1 - p_2 \in Z$ as the additional constraint. Another important case in which the C_2' gives additional constraint is in D_3-insulators, when the C_2' axis coincides with $\mathbf{a}_1$ (or $\mathbf{a}_2$). There the constraint by C_2' symmetry forbids any nontrivial (noninteger) values of p_1 and p_2 to exist. Rows 4 and 5 of Table III list all constraints on (p_1, p_2) for insulators with $D_{n=2,3,4,6}$ invariance on four of the five 2D Braivis lattices. Notice that for D_3-invariant insulators, there are two possible alignment of the C_2' axes in the triangular lattice: either along $\mathbf{a}_1$ (and its C_3 equivalent axes) or along the bisect of $\mathbf{a}_1$ and $\mathbf{a}_2$ (and its C_3 equivalent axes). Applying the constraints, one can easily write down all nontrivial values of $(p_1, p_2) \neq 0$, listed in the last row of Table III. Below each pair of (p_1, p_2), the electronic charge center in the real space lattice is plotted.

A few remarks are due regarding the results shown in Table III. First, we emphasize that all results depend on the vanishing Chern number as a necessary condition, without which the 2D polarization is undefined. Second, although C_2 invariance is a sufficient condition for the vanishing Chern number, it is not necessary for quantization of (p_1, p_2). In other words, given a 2D insulator *with* zero Chern number but *without* C_2' invariance, the constraints placed by C_n shown in the fourth row of Table III are still valid. Third, we notice that for D_3-invariant insulators with C_2' axis aligned with $\mathbf{a}_{1,2}$ or D_6-invariant insulators, $(p_1, p_2) = (0, 0)$ by symmetry, i.e., there is no nontrivial polarization for these insulators.

In Sec. III, we have shown the relation between the Chern number and symmetry eigenvalues at high-symmetry points in BZ. Can we also express the electric polarization (p_1, p_2) in terms of the eigenvalues of symmetry operators in D_n point group at high-symmetry points? To have explicit values of $p_{1,2}$, we need to evaluate the integer q on the right-hand side of Eq. (60), defined through a sewing matrix in Eq. (56). From the definition, we can see that $2\pi q_i(C_n)$ is the phase difference between the determinant of the sewing matrix at two $\mathbf{k}$ points separated by $\mathbf{b}_i$. In principle, q_i depends on i through $\mathbf{b}_i$ and PGS. In practice, due to the presence of constraints, we will see that we only need to calculate $q_1(C_2)$ and $q_1(C_3) - q_2(C_3)$, while all other q's can either be derived or are not needed.

To calculate $q_1(C_2)$, first use its definition in Eq. (56) and the periodicity of the gauge to obtain

$$q_1(C_2) = \frac{-i}{2\pi} \int_{-1/2}^{1/2} dk_1 \frac{d \ln \left\{ \det \left[\mathcal{B}_{C_2}(k_1, 0) \right] \right\}}{dk_1}. \tag{62}$$

In Eq. (62), we have taken $k_2 = 0$ because the integral is k_2 independent. Then we apply the sewing matrix property

Eq. (F3) and have

$$\mathcal{B}_{C_2}(\mathbf{k}) = (-1)^F \mathcal{B}^\dagger_{C_2}(-\mathbf{k}), \tag{63}$$

which leads to

$$\ln\left\{\det\left[B_{C_2}(k_1,0)\right]\right\} = iN_{\rm occ}F\pi - \ln\left\{\det\left[B_{C_2}(-k_1,0)\right]\right\},$$
$$\frac{d\ln\left\{\det\left[B_{C_2}(k_1,0)\right]\right\}}{dk_1} = \frac{d\ln\left\{\det\left[B_{C_2}(-k_1,0)\right]\right\}}{dk_1}. \tag{64}$$

Substitute Eq. (64) into Eq. (62), and we have

$$\begin{aligned} q_1(C_2) &= \frac{-i}{\pi}\int_0^{1/2} dk_1 \frac{d\ln\left\{\det\left[\mathcal{B}_{C_2}(k_1,0)\right]\right\}}{dk_1} \\ &= \frac{-i}{\pi}\ln\left\{\frac{\det\left[\mathcal{B}_{C_2}(X)\right]}{\det\left[\mathcal{B}_{C_2}(\Gamma)\right]}\right\} \mod 2 \\ &= \frac{-i}{\pi}\ln\left[\prod_{n\in\rm occ}\frac{\zeta_n(X)}{\zeta_n(\Gamma)}\right] \mod 2. \end{aligned} \tag{65}$$

Equation (65) can also be put in the form

$$(-1)^{q_1(C_2)} = \prod_{n\in\rm occ}\frac{\zeta_n(X)}{\zeta_n(\Gamma)}. \tag{66}$$

The calculation of q_2 follows exactly the same route only replacing X with Y. The result is

$$(-1)^{q_2(C_2)} = \prod_{n\in\rm occ}\frac{\zeta_n(Y)}{\zeta_n(\Gamma)}. \tag{67}$$

We then use the constraints $2p_1 = q_1(C_2)$ and $2p_2 = q_2(C_2)$ for D_2-invariant insulators to obtain the explicit values of $p_{1,2}$:

$$\begin{aligned} (-1)^{2p_1} &= \prod_{n\in\rm occ}\frac{\zeta_n(X)}{\zeta_n(\Gamma)}, \\ (-1)^{2p_2} &= \prod_{n\in\rm occ}\frac{\zeta_n(Y)}{\zeta_n(\Gamma)}. \end{aligned} \tag{68}$$

Mark that the inversion eigenvalues at M do not enter the formula due to the constraint of vanishing Chern number: $\prod_{i\in\rm occ}\zeta_i(\Gamma)\zeta_i(X)\zeta_i(Y)\zeta_i(M) = 1$.

$q_1(C_2)$ can also be used in calculating p_1 in D_4-invariant insulators, because D_4 already implies D_2. In a D_4-invariant insulator, using the constraint $2p_1 = 2p_2 = q_1(C_2)$ we find

$$(-1)^{2p_{1,2}} = \prod_{n\in\rm occ}\frac{\zeta_n(X)}{\zeta_n(\Gamma)}. \tag{69}$$

To calculate $q_1(C_3)$, we start from inspecting the phase of the determinant of the sewing matrix associated with C_3:

$$\phi(\mathbf{k}) = -i\ln\det\left(\mathcal{B}_{C_3}\right)(\mathbf{k}) \tag{70}$$

in the BZ. Due to the continuous and periodic gauge choice, $\phi(\mathbf{k})$ is a continuous function satisfying

$$\phi(\mathbf{k}+\mathbf{b_i}) = \phi(\mathbf{k}) + 2q_i(C_3)\pi. \tag{71}$$

$\phi(K)$ and $\phi(K')$ can be determined by the C_3 eigenvalues at these two points:

$$\phi(K) = -i\ln\left[\prod_{n\in\rm occ}\theta_n(K)\right], \quad \phi(K') = -i\ln\left[\prod_{n\in\rm occ}\theta_n(K')\right]. \tag{72}$$

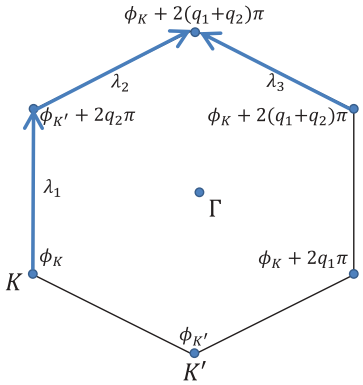


FIG. 3. (Color online) The phase of $\det(\mathcal{B}_{C_3})$ at six corners of the BZ. $\lambda_{1,2,3}$ denote the paths of integration considered in the text.

We can then express $\phi(\mathbf{k})$ at all six corners of the BZ in terms of $\phi(K,K')$ and $q_{1,2}(C_3)$ as shown in Fig. 3. Then we use the sewing matrix property

$$\mathcal{B}_{C_3}(\mathbf{k}) = (-1)^F \mathcal{B}^\dagger_{C_3}(C_3\mathbf{k})\mathcal{B}^\dagger\left(C_3^{-1}\mathbf{k}\right) \tag{73}$$

to have

$$\begin{aligned} &\phi(K') + 2q_2\pi - \phi(K) \\ &= \int_{\lambda_1}\mathrm{Tr}\left[\mathcal{B}_{C_3}(\mathbf{k})\partial\mathcal{B}_{C_3}(\mathbf{k})\right]\cdot d\mathbf{k} \\ &= \left(\int_{\lambda_2} d\mathbf{k} + \int_{\lambda_3} d\mathbf{k}\right)\cdot\mathrm{Tr}\left[\mathcal{B}_{C_3}(\mathbf{k})\partial\mathcal{B}_{C_3}(\mathbf{k})\right] \\ &= 2q_1\pi - 2[\phi(K') - \phi(K)], \end{aligned} \tag{74}$$

where $\lambda_{1,2,3}$ are integration paths marked in Fig. 3. From Eq. (74), we extract

$$q_1(C_3) - q_2(C_3) = \frac{3}{2\pi}[\phi(K') - \phi(K)]. \tag{75}$$

Equation (75) and the constraints placed by C_3 invariance give the final expression of $p_{1,2}$:

$$\exp(i2\pi p_{1,2}) = \prod_{n\in\rm occ}\frac{\theta_n(K)}{\theta_n(K')}. \tag{76}$$

Up to this point, we have formulated the theory of quantized polarization in D_n-invariant insulators. In fact, we emphasize that the theory applies to a wider class of insulators: C_n-invariant insulators with vanishing Chern number. The electric polarization serves as a complimentary quantum number when the Chern number is zero (for example, in D_n-invariant insulators), and just like the Chern number, the electric polarization can be expressed in terms of the C_n eigenvalues of bands at points of symmetry.

V. POINT GROUP SYMMETRIC TOPOLOGICAL INSULATORS IN 3D

In 3D, there exist 32 different point groups, each of which is generated by four types of operators: n-fold rotations C_n, mirror plane reflections M and and rotation-reflection S_n. S_n is a combination of an n-fold rotation followed by a mirror reflection about the plane perpendicular to the rotation axis, or $S_n = C_n * M_{xy}$. In the following, we explore two

fundamental responses of point group symmetric topological insulators: the 3D anisotropic quantum Hall conductance and the magnetoelectric polarization.

A. 3D Anisotropic quantum Hall State

The simplest 3D point groups are the cyclic groups C_n as they are comprised of only one rotation axis, which we assume to be the z axis. The 3D single-particle Hamiltonian $\hat{H}(k_x,k_y,k_z)$ can be constructed from a series of 2D Hamiltonians $\hat{H}_{k_x,k_y;k_z}$, where k_z is a momentum parameter spanning $-\pi$ to π. For every one of these individual 2D systems, one can define a Chern number $C(k_z)$. For an insulator, there is $C(k_z) =$ constant, and if $C(k_z)$ changes at some k_z, there must be, generically, a 3D Weyl node in the bulk.[16–18,32] For $n = 2,3,4,6$, $C(k_z)$ can be calculated using Eqs. (24), (32), (31), and (33), respectively. Each 2D subsystem contributes $\sigma_{xy}(k_z) = Ce^2/h$, and this allows us to easily calculate the total Hall conductance of the 3D system as

$$\sigma_{xy}^{3D} = C(k_z = 0)\frac{e^2 L_z}{ch}, \tag{77}$$

where L_z is the length of the sample in the out-of-plane direction and c is the lattice constant along the the same out-of-plane direction. On the other hand, the other two transverse conductances σ_{xz} and σ_{yz} must be zero as both σ_{xz} and σ_{yz} transform as vectors on xy plane for a rotation about z axis. Therefore they cannot take a nonzero value in a rotation invariant singlet ground state. Based on the preceding argument, as soon as there is more than one rotation axis, all three components of transverse conductance are quantized to zero. This directly applies that D_n, D_{nd}, T_h, T_d, O, and O_h results in $\sigma_{xy} = \sigma_{yz} = \sigma_{xz} = 0$, because they all have at least two rotation axes.

Beyond rotational symmetries, we consider the effect of mirror plane symmetries. For C_{nh} point group, where the mirror plane is perpendicular to the rotation axis (z axis), we can still have a nonzero σ_{xy} given by Eq. (77). For C_{nv} ($n = 2,3,4,6$, while $C_{1v} = C_{1h}$) point group, since the mirror plane is parallel to z axis, $\sigma_{xy} = 0$, because σ_{xy} changes sign under the mirror symmetry while the ground state is a singlet eigenstate invariant under any operation in the point group. As a result, all components of Hall conductance vanish for C_{nv}-invariant insulators.

Finally, we discuss the Spiegel group S_n ($n = 2,4,6$, while S_3 equals C_{3h} and has been discussed). S_2 is the same as inversion, and we borrow the result from Ref. 32, which states that all three transverse conductances may be quantized to nonzero values, depending on the Chern numbers on three planes defined by $k_{i=x,y,z} = 0$, respectively. S_4 and S_6 has C_2 and C_3 as subgroups, respectively, and hence have $\sigma_{xz} = \sigma_{yz} = 0$. To calculate σ_{xy}, we cannot directly apply Eqs. (31) and (33) on $\hat{H}(k_x,k_y;k_z)$ for a generic k_z, because C_4 or C_6 rotational symmetry is not a symmetry of the underlying 2D subsystem. However, the subsystems with $k_z = 0$ or $k_z = \pi$ are invariant under M_{xy} and, on these planes, C_4 or C_6 is restored. The restored rotational invariance allows one to calculate the Chern number on $k_z = 0$ or $k_z = \pi$. The insulating condition requires that the Chern number on every k_z must be the same and the total Hall conductivity, σ_{xy}, is still given by Eq. (77). In fact, the insulating condition requires

$$\prod_{i\in\text{occ}} \frac{\zeta_i(\Gamma)\zeta_i(X)\zeta_i(Y)\zeta_i(S)}{\zeta_i(Z)\zeta_i(U)\zeta_i(T)\zeta_i(R)} = 1, \tag{78}$$

$$\prod_{i\in\text{occ}} \frac{\xi_i(\Gamma)\xi_i(M)\zeta_i(X)}{\xi_i(Z)\xi_i(A)\xi_i(R)} = 1, \tag{79}$$

$$\prod_{i\in\text{occ}} \frac{\eta_i(\Gamma)\theta_i(K)\zeta_i(M)}{\eta_i(A)\theta_i(H)\zeta_i(L)} = 1, \tag{80}$$

for $n = 2,4,6$, respectively.[32] Other values of the above products signal the presence of Weyl fermions.

To summarize our findings concerning the Hall conductance in 3D insulators with point group symmetries, we note that only C_n for $n = 2,3,4$, and 6, C_{nh} ($n = 2,3,4,6$) and S_n ($n = 2,4,6$) can have nonzero Hall conductance quantized to a multiple of the number of layers along the third direction. 3D insulators with any other point group symmetry must have $\sigma_{xy} = \sigma_{yz} = \sigma_{xz} = 0$. In particular, with the exception of S_2, or 3D inversion, which is compatible with nonzero σ_{xz} and σ_{yz}, all point group symmetric topological insulators have vanishing σ_{xz} and σ_{yz}, assuming z axis to be the principle axis.

B. Magnetoelectric Effect

It is known that topological insulators with time-reversal *or* space-inversion symmetry in 3D posses a coefficient of the magnetoelectric term $\mathbf{E}\cdot\mathbf{B}$, P_3, which must be quantized to either zero or one-half.[23,32,33] We now desire to find if P_3 is quantized in the presence of a general PGS in a 3D insulator. We begin our discussion by considering the magnetoelectric effect in a 3D topological insulator with an arbitrary rotation symmetry, the operator of which is denoted by $\hat{R}$. In 3D, a rotation R can either be a *proper* or an *improper* rotation. In a proper rotation, the system is rotated about a given axis in space by a given angle; while in an improper rotation is the combination of a proper rotation and space inversion, i.e., $(x,y,z) \to (-x,-y,-z)$. Mathematically, if R_{ij} is the three-by-three rotation matrix, then $\det(R) = 1$ for proper rotations and $\det(R) = -1$ for improper rotations. A general operation in a point group is either a proper or an improper rotation.

Before discussing the quantization of P_3, readers are reminded that $P_3\mathbf{E}\cdot\mathbf{B}$ is *not* the only magnetoelectric response term in the Hamiltonian, It has been shown that in general there exists a cross-gap contribution, P^o_{ij}, a real tensor, and the total response should be $P^o_{ij}E_iB_j + P_3\mathbf{E}\cdot\mathbf{B}$.[38,39] In any insulators with time-reversal *or* space inversion symmetry, P^o_{ij} is proved to be zero, which is why it is sometimes neglected, and this quantity also vanishes in the flat band limit, where all occupied bands have the same energy and all unoccupied bands have the same energy. Therefore, unlike P_3, P^o_{ij} is *not* a quantized/topological quantity so therefore does not concern our major interest in this paper. However, we find that PGS places strong constraints on the components of P^o_{ij}, which is detailed in Appendix G.

By Eq. (12), one can use $\mathcal{B}(\mathbf{k})$ to express $|u(\mathbf{k}')\rangle$ in terms of $\hat{R}|u(\mathbf{k})\rangle$, where $\mathbf{k}' = R\mathbf{k}$ is $\mathbf{k}$ transformed by R:

$$|u_a(\mathbf{k}')\rangle = \sum_{b\in\text{occ}} \mathcal{B}^{\star}_{ab}(\mathbf{k})\hat{R}|u_b(\mathbf{k})\rangle. \tag{81}$$

Using Eq. (81), the non-Abelian Berry connection $\mathcal{A}_i(k)$ then has the following property:

$$\begin{aligned}(\mathcal{A}_i(\mathbf{k}^{'}))_{ab} &= -i\langle u_a(\mathbf{k}^{'})|R_{ij}\partial_j|u_b(\mathbf{k}^{'})\rangle \\ &= -iR_{ij}\sum_{c,d\in\text{occ}}\mathcal{B}_{ac}(\mathbf{k})\langle u_c(\mathbf{k})|\hat{R}^{-1}\partial_j\mathcal{B}^{\star}_{bd}(\mathbf{k})\hat{R}|u_d(\mathbf{k})\rangle \\ &= -iR_{ij}\sum_{c,d\in\text{occ}}\mathcal{B}_{ac}(\mathbf{k})\langle u_c(\mathbf{k})|\partial_j\mathcal{B}^{\star}_{bd}(\mathbf{k})|u_d(\mathbf{k})\rangle \\ &= R_{ij}(\mathcal{B}(\mathbf{k})\mathcal{A}_j(\mathbf{k})\mathcal{B}^{-1}(\mathbf{k}))_{ab} - iR_{ij}(\mathcal{B}(\mathbf{k})\partial_j\mathcal{B}(\mathbf{k}))_{ab}.\end{aligned} \tag{82}$$

This non-Abelian gauge transformation exactly takes the form of the non-Ableian transform of a gauge potential, with the exception of the presence of the prefactor R_{ij}. The transformation of the field strength, whose proof is included in Appendix E, is

$$\mathcal{F}_{ij}(\mathbf{k}^{'}) = R_{ii'}R_{jj'}\mathcal{B}(\mathbf{k})\mathcal{F}_{i'j'}(\mathbf{k})\mathcal{B}^{\dagger}(\mathbf{k}). \tag{83}$$

We are now in a favorable position to understand the constraints on P_3 imposed by the presence of general rotation symmetry R. In fact, one has

$$\begin{aligned}n+P_3 &= \frac{1}{16\pi^2}\int d^3k\epsilon_{ijk}\text{Tr}\left\{\left[\mathcal{F}_{ij}(\mathbf{k})-\frac{2}{3}i\mathcal{A}_i(\mathbf{k})\mathcal{A}_j(\mathbf{k})\right]\mathcal{A}_k(\mathbf{k})\right\} = \frac{1}{16\pi^2}\int d^3k'\epsilon_{ijk}\text{Tr}\left\{\left[\mathcal{F}_{ij}(\mathbf{k}')-\frac{2}{3}i\mathcal{A}_i(\mathbf{k}')\mathcal{A}_j(\mathbf{k}')\right]\mathcal{A}_k(\mathbf{k}')\right\} \\ &= \frac{1}{16\pi^2}\int d^3k\epsilon_{ijk}R_{ii'}R_{jj'}R_{kk'}\text{Tr}\left\{\left[\mathcal{B}\mathcal{F}_{i'j'}\mathcal{B}^{\dagger}-\frac{2i}{3}(\mathcal{B}\mathcal{A}_{i'}\mathcal{B}^{\dagger}-i\mathcal{B}\partial_{i'}\mathcal{B}^{\dagger})(\mathcal{B}\mathcal{A}_{j'}\mathcal{B}^{\dagger}-i\mathcal{B}\partial_{j'}\mathcal{B}^{\dagger})\right](\mathcal{B}\mathcal{A}_{k'}\mathcal{B}^{\dagger}-i\mathcal{B}\partial_{k'}\mathcal{B}^{\dagger})\right\},\end{aligned} \tag{84}$$

where n is a gauge dependent degree of freedom. To proceed, notice that

$$\epsilon_{ijk}R_{ii'}R_{jj'}R_{kk'} = \det(R)\epsilon_{i'j'k'} = \pm\epsilon_{i'j'k'}. \tag{85}$$

If R is a proper rotation plus sign is taken and if R is an improper minus sign is taken. Then we have

$$\begin{aligned}n+P_3 &= \frac{\pm}{16\pi^2}\int d^3k\epsilon_{ijk}\text{Tr}\left\{\left[\mathcal{B}\mathcal{F}_{ij}B^{\dagger}-\frac{2i}{3}(B\mathcal{A}_i\mathcal{B}^{\dagger}-i\mathcal{B}\partial_i\mathcal{B}^{\dagger})(\mathcal{B}\mathcal{A}_j\mathcal{B}^{\dagger}-i\mathcal{B}\partial_j\mathcal{B}^{\dagger})\right](\mathcal{B}\mathcal{A}_k\mathcal{B}^{\dagger}-i\mathcal{B}\partial_k\mathcal{B}^{\dagger})\right\} \\ &= \frac{\pm}{16\pi^2}\int d^3k\epsilon_{ijk}\text{Tr}\left[\left(\mathcal{F}_{ij}-\frac{2}{3}i\mathcal{A}_i\mathcal{A}_j\right)\mathcal{A}_k\right]+\frac{1}{24\pi^2}\int d^3k\text{Tr}[(\mathcal{B}\partial_i\mathcal{B}^{\dagger})(\mathcal{B}\partial_j\mathcal{B}^{\dagger})(\mathcal{B}\partial_k\mathcal{B}^{\dagger})]-\frac{i}{8\pi^2}\int d^3k\epsilon_{ijk}\partial_i[\text{Tr}(\mathcal{B}\mathcal{A}_j\partial_k\mathcal{B}^{\dagger})] \\ &= \pm(n+P_3)\pm\frac{1}{24\pi^2}\int d^3k\text{Tr}[(\mathcal{B}\partial_i\mathcal{B}^{\dagger})(\mathcal{B}\partial_j\mathcal{B}^{\dagger})(\mathcal{B}\partial_k\mathcal{B}^{\dagger})].\end{aligned} \tag{86}$$

If R is improper, we have

$$P_3 = \frac{-1}{48\pi^2}\int d^3k\epsilon_{ijk}\text{Tr}[(\mathcal{B}\partial_i\mathcal{B}^{\dagger})(\mathcal{B}\partial_j\mathcal{B}^{\dagger})(\mathcal{B}\partial_k\mathcal{B}^{\dagger})] \text{ mod } 1, \tag{87}$$

which is indeed one half of the winding number of B. However, if R is proper, the two P_3's cancel each other and the symmetry has no constraint on P_3. Additionally, it gives

$$\frac{1}{24\pi^2}\int d^3k\text{Tr}[(\mathcal{B}\partial_i\mathcal{B}^{\dagger})(\mathcal{B}\partial_j\mathcal{B}^{\dagger})(\mathcal{B}\partial_k\mathcal{B}^{\dagger})] = 0. \tag{88}$$

Equation (88) indicates that although one may define the winding number of the sewing matrix as a quantum number, that number is always zero.

Up to this point, we have formally derived the statement that only systems with improper rotation symmetry can have quantized P_3. In fact, there is a simple way to understand this simple result. In an insulating medium with applied electromagnetic field, any point group symmetry of the medium must be preserved if one rotates the applied field together, which means that the axion term in the Hamiltonian density $P_3\mathbf{E}\cdot\mathbf{B}$ remains invariant under some improper symmetry. On the other hand, since $\mathbf{E}\cdot\mathbf{B}$ is a *pseudoscalar*, under any improper rotation there is $\mathbf{E}\cdot\mathbf{B}\rightarrow-\mathbf{E}\cdot\mathbf{B}$. Therefore we have $P_3 = -P_3$. From this equation, one may be tempted to obtain $P_3 = 0$, but is reminded that P_3 is only well defined up to some integer in a compact space. Therefore $P_3 = -P_3$ should be interpreted as $P_3 = -P_3 +$ integer or $2P_3 =$ integer. This is the intuitive argument leading to the same quantization of P_3 in insulators having some improper rotation symmetry.

It is easy to check that every point group that contains an improper rotation operation must have any of C_s, S_2, or S_4 as its subgroup(s), where C_s is a group generated by just one mirror plane. Therefore the smallest symmetry point groups that have quantized P_3 are C_s, S_2 and S_4, where it should be noted that S_2 is *not* a subgroup of S_4. But this does not tell us whether it is possible to have P_3 quantized to the nontrivial value of $1/2$ in the presence of C_s, S_2 and S_4. In Refs. 32 and 33, it was made clear that there are insulators having inversion invariance without time-reversal invariance that still have nontrivial P_3. In the following, we will give examples of systems having only C_s or only S_4 that have nontrivial P_3. We begin with a 3D Hamiltonian

$$\mathcal{H}(\mathbf{k}) = \sin(k_x)\Gamma_1+\sin(k_y)\Gamma_2+\sin(k_z)\Gamma_z+M(\mathbf{k})\Gamma_0, \tag{89}$$

where $M(\mathbf{k}) = 3-m-\cos(k_x)-\cos(k_y)-\cos(k_y)$, $\Gamma_0 = 1\otimes\tau_z$, $\Gamma_1 = \sigma_z\otimes\tau_x$, $\Gamma_2 = 1\otimes\tau_y$, and $\Gamma_3 = \sigma_y\otimes\tau_x$. This Hamiltonian has time-reversal symmetry and O_h point group symmetry. One can add terms to break it down to smaller point groups. To do so, we add a magnetic field along z axis and an

electric field along x axis:

$$\delta\mathcal{H} = B\Gamma_{35} + E\Gamma_{10}. \tag{90}$$

The magnetic field breaks time reversal symmetry and all rotation axes except those about the z axis, while the electric field further breaks rotation symmetry about z axis. The only symmetry remaining is the mirror reflection about xy plane. On the other hand, P_3 must remain unchanged in so much as the external fields are not so strong as to close the bulk gap, because a mirror reflection is still an improper rotation and quantizes P_3. If we choose the parameter $0 < m < 3$, we obtain a 3D model that has $P_3 = 1/2$ but no symmetry other than a reflection about xy plane or point group C_s. We can also add the term

$$\delta\mathcal{H}_2(\mathbf{k}) = B\Gamma_{35} + t\sin(k_x)\Gamma_{15} - t\sin(k_y)\Gamma_{25} \tag{91}$$

to our 3D Hamiltonian. In Eq. (91), the first term removes time-reversal symmetry and all rotation axes except z axis, while the second term breaks both C_4 and M_z separately but preserves their combination $S_4 = C_4 * M_{xy}$. As before, as long as the added terms are not large enough to close the bulk gap, P_3 remains quantized at $n + 1/2$ if $0 < m < 3$.

While time-reversal symmetry is not the major topic of the paper, it is still interesting to discuss how this symmetry can change the previous results. Intuitively, since time-reversal operation T, like inversion, sends $\mathbf{k}$ to $-\mathbf{k}$, it is similar to an improper rotation symmetry as far as P_3 is concerned. Generally, a symmetry operation $T * R$ is equivalent to an improper/proper rotation if R is a proper/improper rotation. Therefore P_3 is quantized when TR is a symmetry of the system for some proper R. From the statement, also a not very obvious result is derived: if the system is *not* invariant under separate inversion (P) or time-reversal (T), but is invariant under their combined operation ($P * T$), it does *not* have quantized P_3, as $P * T$ is proper.[38,39]

VI. CONCLUSION

We study several bulk topological invariants in 2D and 3D insulators with crystallographic point group symmetries, focusing on finding (i) the constraints placed by these symmetries on known topological invariants such as the Chern number and (ii) if a PGS gives rise to new topological invariants. In 2D, we show that the Chern numbers of a C_n invariant insulator are determined up to a multiple of n by eigenvalues of C_m at high-symmetry points, where m divides n. In D_n-invariant insulators, we show that the Chern number is constrained to be zero, while the electric polarization, or the center of charge position is a new topological invariant, the value of which can be determined by eigenvalues of C_m at high-symmetry points, where m divides n. In 3D, we show that only C_n, C_{nh}, and S_n invariant insulators can have nonzero anisotropic 3D quantum Hall conductance, while insulators with all other point group symmetries must have zero Hall conductance in every component. We also prove that the magnetoelectric susceptibility of point group symmetric topological insulators in 3D is quantized to 0 or $1/2$, i.e., a Z_2 number, if and only if the point group contains at least one improper rotation.

Note added. Recently, we became aware of another work by R. Slager, A. Mesaros, V. Juricis, and J. Zaanen[40] on classification of topological insulators with space group and time-reversal symmetry.

ACKNOWLEDGMENTS

M.J.G. acknowledges support from the AFOSR under grant FA9550-10-1-0459 and the ONR under grant N0014-11-1-0728 and a gift the Intel Corporation. B.A.B. was supported by NSF CAREER DMR-095242, ONR N00014-11-1-0635, Darpa N66001-11-1-4110, and David and Lucile Packard Foundation. M.J.G. and B.A.B. thank the Chinese Academy of Sciences for generous hosting; B.A.B. thanks Microsoft Station Q for generous hosting.

APPENDIX A: DETAILS IN EQ. (29)

In Eq. (29), we showed how the determinant of a Wilson loop enclosing a quarter of the BZ ($\lambda = \Gamma XMY\Gamma$) can be expressed in terms of the sewing matrices, but omitted several steps in which identity operators are inserted. The full details are given here:

$$\begin{aligned}
&\det[\langle u_i(\Gamma)|\tilde{U}_\lambda|u_j(\Gamma)\rangle] \\
&= \det[\langle u_i(\Gamma)|\tilde{U}_{\Gamma X}\tilde{U}_{XM}\tilde{U}_{MY}\tilde{U}_{Y\Gamma}|u_j(\Gamma)\rangle] = \det\left[\langle u_i(\Gamma)|\tilde{C}_4\left(\tilde{C}_4^{-1}\tilde{U}_{\Gamma X}\tilde{C}_4\right)\tilde{C}_2^{-1}\left(\tilde{C}_4\tilde{U}_{XM}\tilde{C}_4^{-1}\right)\tilde{C}_4\tilde{U}_{MY}\tilde{U}_{Y\Gamma}|u_j(\Gamma)\rangle\right] \\
&= \det\left[\langle u_i(\Gamma)|\tilde{C}_4\tilde{U}_{\Gamma Y}\tilde{C}_2^{-1}\tilde{U}_{YM}\tilde{C}_4\tilde{U}_{MY}\tilde{U}_{Y\Gamma}|u_j(\Gamma)\rangle\right] \\
&= \det[\sum_{a,b,c,d,e,f\in\text{occ}} \langle u_i(\Gamma)|\tilde{C}_4|u_a(\Gamma)\rangle\langle u_a(\Gamma)|\tilde{U}_{\Gamma Y}|u_b(Y)\rangle\langle u_b(Y)|\tilde{C}_2|u_c(Y)\rangle\langle u_c(Y)|\tilde{U}_{YM}|u_d(M)\rangle \\
&\quad\times\langle u_d(M)|\tilde{C}_4|u_e(M)\rangle\langle u_e(M)|\tilde{U}_{MY}|u_f(Y)\rangle\langle u_f(Y)|\tilde{U}_{Y\Gamma}|u_j(\Gamma)\rangle] = \det\left[\mathcal{B}_{C_4}(\Gamma)\mathcal{U}_{\Gamma Y}\mathcal{B}_{C_2}^{-1}(Y)\mathcal{U}_{YM}\mathcal{B}_{C_4}(M)\mathcal{U}_{MY}\mathcal{U}_{Y\gamma}\right] \\
&= \det\left[\mathcal{B}_{C_4}(\Gamma)\mathcal{B}_{C_2}^{-1}(Y)\mathcal{B}_{C_4}(M)\right]\det(\mathcal{U}_{\Gamma Y}\mathcal{U}_{YM}\mathcal{U}_{MY}\mathcal{U}_{Y\Gamma}) = \det\left[\mathcal{B}_{C_4}(\Gamma)\mathcal{B}_{C_2}^{-1}(Y)\mathcal{B}_{C_4}(M)\right].
\end{aligned} \tag{A1}$$

In the steps, we notice that we insert operators like $\sum_{a\in\text{occ}}|u_a(\mathbf{k})\rangle\langle u_a(\mathbf{k})|$ as identity operators, which is allowed if and only if C_4 is a symmetry of the system and the system is fully gapped. The C_4 symmetry guarantees the existence of another band of equal energy at $C_4\mathbf{k}$ while the insulating gap guarantees no mixing from the unoccupied bands.

APPENDIX B: PROOF BY MONODROMY WITH C_3 AND C_6 SYMMETRIES

In this appendix, we prove the Eqs. (32) and (33) using monodromy argument. For C_3 invariant systems, choose a loop shown in Fig. 1(c). From C_3 symmetry, we have [through Eq.(83)] $\mathcal{F}_{xy}(\mathbf{k}) = \mathcal{F}_{xy}(R_3\mathbf{k})$ and therefore the determinant of the loop integral shown in Fig. 1(c) is

$$\det(\mathcal{U}_\lambda) = e^{i2C\pi/3}, \tag{B1}$$

where $(\mathcal{U}_\lambda)_{ij} = \langle u_i(\Gamma)|\tilde{U}_\lambda|u_j(\Gamma)\rangle$. Again using C_3 symmetry we notice that, using Eq. (23), $\tilde{C}_3^{-1}\tilde{U}_{\Gamma K''}\tilde{C}_3 = \tilde{U}_{\Gamma K'}$ and $\tilde{C}_3\tilde{U}_{K''K}\tilde{C}_3^{-1} = \tilde{U}_{K'K}$, which leads to

$$\begin{aligned}\tilde{U}_\lambda &= \tilde{U}_{\Gamma K''}\tilde{U}_{K''K}\tilde{U}_{KK'}\tilde{U}_{K'\Gamma}\\ &= \tilde{U}_{\Gamma K''}\tilde{U}_{K''K}\tilde{C}_3\tilde{U}_{KK''}\tilde{C}_3^{-1}\tilde{C}_3^{-1}\tilde{U}_{K''\Gamma}\tilde{C}_3.\end{aligned} \tag{B2}$$

After inserting identity operators as done in Eq. (A1), the determinant $\det\mathcal{U}_\lambda$ simplifies as

$$\begin{aligned}\det(\mathcal{U}_\lambda) &= \det[\mathcal{U}_{\Gamma K''}\mathcal{U}_{K''K}\mathcal{B}(K)\mathcal{U}_{KK''}\mathcal{B}^{-2}(K'')\mathcal{U}_{K''\Gamma}\mathcal{B}(\Gamma)]\\ &= \det[\mathcal{B}(K)\mathcal{B}^{-2}(K')\mathcal{B}(\Gamma)].\end{aligned} \tag{B3}$$

In the derivation, we have noticed that K' and K'' are the same point by translational symmetry. Then using $\mathcal{B}^3 = (-1)^F\mathcal{I}_{N_{\rm occ}\times N_{\rm occ}}$ on Eq. (B3) and combining Eq. (B1), we have

$$e^{i2C\pi/3} = \prod_{i\in{\rm occ}}(-1)^F\theta_i(\Gamma)\theta_i(K)\theta_i(K'). \tag{B4}$$

For C_6, we consider the loop shown in Fig. 1(d). The determinant of its loop integral is

$$\det(\mathcal{U}_\lambda) = e^{iC\pi/3}. \tag{B5}$$

Notice that $\tilde{C}_6^{-1}\tilde{U}_{\Gamma M}\tilde{C}_6 = \tilde{U}_{\Gamma M'}$ and $\tilde{C}_3\tilde{U}_{MK}\tilde{C}_3^{-1} = \tilde{U}_{M'K}$, and we have

$$\begin{aligned}\tilde{U}_\lambda &= \tilde{U}_{\Gamma M}\tilde{U}_{MK}\tilde{U}_{KM'}\tilde{U}_{M'\Gamma}\\ &= \tilde{U}_{\Gamma M}\tilde{U}_{MK}\tilde{C}_3\tilde{U}_{KM}\tilde{C}_3^{-1}\tilde{C}_6^{-1}\tilde{U}_{M\Gamma}\tilde{C}_6.\end{aligned} \tag{B6}$$

Inserting identity operators, the determinant becomes

$$\begin{aligned}\det(\mathcal{U}_\lambda) &= \det\left[\mathcal{U}_{\Gamma M}\mathcal{U}_{MK}\mathcal{B}_{C_3}(K)\mathcal{U}_{KM}\mathcal{B}_{C_2}^{-1}(M)\mathcal{U}_{M\Gamma}\mathcal{B}_{C_6}(\Gamma)\right]\\ &= \det\left[\mathcal{B}_{C_6}(\Gamma)\mathcal{B}_{C_3}(K)\mathcal{B}_{C_2}^{-1}\right],\end{aligned} \tag{B7}$$

where we have used that $C_3 * C_6 = C_2$. Noticing that $\tilde{C}_2^2 = (-1)^F$, we obtain

$$e^{iC\pi/3} = \prod_{i\in{\rm occ}}(-1)^F\eta_i(\Gamma)\theta_i(K)\zeta_i(K'). \tag{B8}$$

APPENDIX C: HIGH-SYMMETRY POINTS IN A FINITE SYSTEM

In Sec. III B, we have derived the relation between the many-body C_n eigenvalue and the C_m (m dividing n) eigenvalues at high-symmetry points in the BZ, upon the condition that all these points can be taken in our system. In a real system, whether a $\mathbf{k}$ point appears on the grid depends on the total number of unit cells along each direction. For example, in a 1D system, $k = \pi$ only appears when there are even number of unit cells. In this appendix, we exhaust the possibilities of the presence/absence of each high-symmetry point in a 2D system.

On a 2D lattice with periodic boundary, a point on the grid can be generally written as

$$\mathbf{k} = \frac{2\pi(n_1-1)}{N_1}\mathbf{b}_1 + \frac{2\pi(n_2-1)}{N_2}\mathbf{b}_2, \tag{C1}$$

where $n_1 = 1,\ldots,N_1$ and $n_2 = 1,\ldots,N_2$. For each high-symmetry point, the corresponding (n_1,n_2) are given by

$\Gamma : (n_1,n_2) = (1,1),\ X : (n_1,n_2) = (N_1/2,1),\ Y : (n_1,n_2) = (1,N_2/2),\ M : (n_1,n_2) = (N_1/2,N_2/2)$ for $n = 2,4$;
$K : (n_1,n_2) = (N_1/3,2N_2/3),\ K' : (n_1,n_2) = (2N_1/3,N_2/3)$ for $n = 3,6$.

Therefore the parity of $N_{1,2}$ determines whether a certain high-symmetry point can exist in the system. For $n = 3,4,6$, we also implicitly assume that $N_1 = N_2 = N_0$, because otherwise the many-body system cannot have the corresponding symmetries.

Disappearance of high-symmetry points changes the results in Sec. III B in two aspects. First, one must remove the C_m eigenvalues at those points from the formulas; second, there are more $\mathbf{k}$ points grouped into groups of two, three, four, and six, respectively, which requires correction of the prefactors in, for example, Eqs. (38), (45), and (47). Below we rewrite the formulas for different combinations of parities of N_1 and N_2.

For $n = 2$, if $N_1 =$ even and $N_2 =$ odd,

$$\hat{C}_2|\Phi_0\rangle = (-1)^{\frac{(F-1)N_{\rm occ}(N-2)}{2}}\prod_{i\in{\rm occ}}\zeta_i(\Gamma)\zeta_i(X)|\Phi_0\rangle, \tag{C2}$$

if $N_1 =$ odd and $N_2 =$ even,

$$\hat{C}_2|\Phi_0\rangle = (-1)^{\frac{(F-1)N_{\rm occ}(N-2)}{2}}\prod_{i\in{\rm occ}}\zeta_i(\Gamma)\zeta_i(Y)|\Phi_0\rangle, \tag{C3}$$

if $N_1 =$ odd and $N_2 =$ odd,

$$\hat{C}_2|\Phi_0\rangle = (-1)^{\frac{(F-1)N_{\rm occ}(N-1)}{2}}\prod_{i\in{\rm occ}}\zeta_i(\Gamma)|\Phi_0\rangle. \tag{C4}$$

For $n = 3$, if $N_0 \bmod 3 \neq 0$,

$$\hat{C}_3|\Phi_0\rangle = (-1)^{FN_{\rm occ}(N-1)/3}\prod_{i\in{\rm occ}}\theta_i(\Gamma)|\Phi_0\rangle. \tag{C5}$$

For $n = 4$, if $N_0 =$ odd,

$$\hat{C}_4|\Phi_0\rangle = (-1)^{(F-1)N_{\rm occ}(N-1)/4}\prod_{i\in{\rm occ}}\xi_i(\Gamma)|\Phi_0\rangle. \tag{C6}$$

For $n = 6$, if $N_0 =$ even and $N_0 \bmod 3 \neq 0$,

$$\hat{C}_6|\Phi_0\rangle = (-1)^{(F-1)N_{\rm occ}(N-4)/6}\prod_{i\in{\rm occ}}\eta_i(\Gamma)\zeta_i(M)|\Phi_0\rangle, \tag{C7}$$

if $N_0 =$ odd and $N_0 \bmod 3 = 0$,

$$\hat{C}_6|\Phi_0\rangle = (-1)^{(F-1)N_{\rm occ}(N-3)/6}\prod_{i\in{\rm occ}}\eta_i(\Gamma)\theta_i(K)|\Phi_0\rangle, \tag{C8}$$

if $N_0 =$ odd and $N_0 \bmod 3 \neq 0$,

$$\hat{C}_6|\Phi_0\rangle = (-1)^{(F-1)N_{\rm occ}(N-1)/6} \prod_{i\in{\rm occ}} \eta_i(\Gamma). \tag{C9}$$

APPENDIX D: VANISHING COMPONENTS OF HALL CONDUCTANCE IN PRESENCE OF CERTAIN POINT GROUP SYMMETRIES

With point group symmetries, some components of Hall conductance are necessarily zero. There are three components of Hall conductance σ_{xz}, σ_{yz} and σ_{xy}. By definition, we have $j_a = \sigma_{ab}E_b$. Under rotation $R : r_a = R_{ab}r'_b$, we have

$$R_{ab}j'_b = \sigma_{ab}R_{bc}E'_c, \tag{D1}$$

or

$$j'_a = (R^{-1}\sigma R)_{ab}E'_b. \tag{D2}$$

In terms of quantum operators, this means

$$\hat{R}^{-1}\hat{\sigma}_{ab}\hat{R} = R^{-1}_{aa'}\hat{\sigma}_{a'b'}R_{b'b}, \tag{D3}$$

where

$$\hat{\sigma}_{ab} \equiv \lim_{\omega\to 0}\frac{1-e^{-\beta\omega}}{2\omega}\int_{-\infty}^{\infty}\hat{j}_a(t)\hat{j}_b(0)e^{i\omega t}dt. \tag{D4}$$

Specially, if R is an n-fold rotation about z axis, we have

$$\begin{aligned}\hat{R}^{-1}\hat{\sigma}_{xz}\hat{R} &= \cos(2\pi/n)\hat{\sigma}_{xz} - \sin(2\pi/n)\hat{\sigma}_{yz},\\ \hat{R}^{-1}\hat{\sigma}_{yz}\hat{R} &= \cos(2\pi/n)\hat{\sigma}_{yz} + \sin(2\pi/n)\hat{\sigma}_{xz}.\end{aligned} \tag{D5}$$

Now we consider an insulating system with n-fold symmetry, and we further assume that the ground state is *nondegenerate*, we have $\hat{R}|\Phi_0\rangle = \lambda(R)|\Phi_0\rangle$, because a nondegenerate ground state must be a 1D representation of the symmetry. It can be easily proved that $\sigma_{xz} = \sigma_{yz} = 0$:

$$\begin{aligned}\sigma_{xz} &= \langle\Phi_0|\hat{\sigma}_{xz}|\Phi_0\rangle\\ &= \frac{1}{n}\sum_{i=0,\ldots,n-1}\langle\Phi_0|\hat{R}^i\hat{R}^{-i}\hat{\sigma}_{xz}\hat{R}^i\hat{R}^{-i}|\Phi_0\rangle\\ &= \frac{1}{n}\sum_{i=0,\ldots,n-1}\left[\cos\left(\frac{2\pi i}{n}\right)\sigma_{xz} - \sin\left(\frac{2\pi i}{n}\right)\sigma_{yz}\right]\\ &= 0,\end{aligned} \tag{D6}$$

in which we have used $\lambda^*_R\lambda_R = 1$ and the mathematical identity $\sum_{i=0,\ldots,n-1}\cos\frac{2\pi i}{n} = \sum_{i=0,\ldots,n-1}\sin\frac{2\pi i}{n} = 0$. Specially, we have that in a 3D system with more than one rotation axis, $\sigma_{xz} = \sigma_{yz} = \sigma_{xy} = 0$; and in a 2D system with mirror symmetry, $\sigma_{xy} = 0$, because the mirror symmetry can be seen as a two-fold rotation about an in-plane axis.

Mark that this proof only uses the definition of Hall conductance and that the many-body ground state is a singlet. The conclusion applies to any interacting system with a singlet ground state.

For $n =$ even, there exists a simpler proof utilizing the fact that any D_n-symmetric 2D insulator must have zero Chern number. If the system is invariant under an even-fold rotation about z axis, it must also be invariant under a twofold rotation about z axis. Therefore the 2D plane in $\mathbf{k}$ space defined by $k_x = 0$ is a 2D insulator with at least D_1 symmetry, therefore, $\sigma_{yz}(k_x = 0) = 0$. Then since the quantized $\sigma_{yz}(k_x)$ must be smooth in an insulator, it must be a constant. Hence $\sigma_{yz}(k_x) = 0$ for each k_x and finally, the total $\sigma_{yz} = 0$.

APPENDIX E: TRANSFORM OF FIELD STRENGTH $\mathcal{F}$ UNDER POINT GROUP SYMMETRY R [PROVING EQ. 83]

$$\mathcal{F}_{ij}(\mathbf{k}) = \partial_i\mathcal{A}_j(\mathbf{k}) - \partial_j\mathcal{A}_i(\mathbf{k}) + i[\mathcal{A}_i(\mathbf{k}),\mathcal{A}_j(\mathbf{k})], \tag{E1}$$

and we look at the Abelian and non-Abelian terms separately, using Eq. (82):

$$\begin{aligned}\partial_i\mathcal{A}_j(\mathbf{k}') - \partial_j A_i(\mathbf{k}') &= R_{ii'}R_{jj'}[\partial_{i'}(\mathcal{B}\mathcal{A}_{j'}\mathcal{B}^\dagger - i\mathcal{B}\partial_{j'}\mathcal{B}^\dagger) - \partial_{j'}(\mathcal{B}\mathcal{A}_{i'}\mathcal{B}^\dagger - i\mathcal{B}\partial_{i'}\mathcal{B}^\dagger)]\\ &= R_{ii'}R_{jj'}\mathcal{B}(\partial_{i'}\mathcal{A}_{j'} - \partial_{j'}\mathcal{A}_{i'})\mathcal{B}^\dagger + R_{ii'}R_{jj'}[(\partial_{i'}\mathcal{B})\mathcal{A}_{j'}\mathcal{B}^\dagger + \mathcal{B}\mathcal{A}_{j'}(\partial_{i'}\mathcal{B}^\dagger) - (\partial_{j'}\mathcal{B})\mathcal{A}\mathcal{B}^\dagger - \mathcal{B}\mathcal{A}_{i'}\partial_{j'}\mathcal{B}^\dagger]\\ &\quad - iR_{ii'}R_{jj'}(\partial_{i'}\mathcal{B}\partial_{j'}\mathcal{B}^\dagger - \partial_{j'}\mathcal{B}\partial_{i'}\mathcal{B}^\dagger),\end{aligned} \tag{E2}$$

$$\begin{aligned}[\mathcal{A}_i(\mathbf{k}'),\mathcal{A}_j(\mathbf{k}')] &= R_{ii'}R_{jj'}[\mathcal{B}\mathcal{A}_{i'}\mathcal{B}^\dagger - i\mathcal{B}\partial_{i'}\mathcal{B}^\dagger, \mathcal{B}\mathcal{A}_{j'}\mathcal{B}^\dagger - i\mathcal{B}\partial_{j'}\mathcal{B}^\dagger]\\ &= R_{ii'}R_{jj'}\mathcal{B}[\mathcal{A}_{i'},\mathcal{A}_{j'}]\mathcal{B}^\dagger - iR_{ii'}R_{jj'}(\mathcal{B}\mathcal{A}_{i'}\partial_{j'}\mathcal{B}^\dagger + (\partial_{j'}\mathcal{B})\mathcal{A}_{i'}\mathcal{B}^\dagger - iR_{ii'}R_{jj'}(\partial_{i'}\mathcal{B}\mathcal{A}_{j'}\mathcal{B}^\dagger + \mathcal{B}\mathcal{A}_{j'}\partial_{i'}\mathcal{B}^\dagger)\\ &\quad + R_{ii'}R_{jj'}(\partial_{i'}\mathcal{B}\partial_{j'}\mathcal{B}^\dagger - \partial_{j'}\mathcal{B}\partial_{i'}\mathcal{B}^\dagger).\end{aligned} \tag{E3}$$

From these two equations, Eq. (83) directly follows. (In the above expressions the argument of $\mathbf{k}$ is suppressed while that of $\mathbf{k}'$ is kept explicit.)

APPENDIX F: BASIC PROPERTIES OF THE SEWING MATRIX

Every point group symmetry operation has a certain order, i.e., there exists integer $n(R)$ for which $R^{n(R)} = E$ or

$R^{n(R)} = E'$, where E and E' are identity operation and a 2π rotation, respectively. The distinction between E and E' is necessary as we are interested in the representation in Hilbert space of a single fermion. For fermions with integer spins, the representation of both E and E' are $\hat{I}$, but for fermions with half-integer spins, the representation for E and E' are $\hat{I}$ and $-\hat{I}$, respectively. For a sewing matrix associated with a point group symmetry R with order n, we have

$$\begin{aligned}&\left[\prod_{s=0,\ldots,n-1}\mathcal{B}(R^s\mathbf{k})\right]_{ij}\\&=\sum_{i_1,i_2,\ldots,i_n\in\mathrm{occ}}\langle u_i(R^n\mathbf{k})|\tilde{R}|u_{i_{n-1}}(R^{n-1}\mathbf{k})\rangle\\&\quad\times\langle u_{i_{n-1}}(R^{n-1}\mathbf{k})|\tilde{R}|u_{i_{n-2}}(R^{n-2}\mathbf{k})\rangle\ldots\langle u_{i_2}(R\mathbf{k})|\tilde{R}|u_j(\mathbf{k})\rangle\\&=\langle u_i(R^n\mathbf{k})|\tilde{R}^n|u_j(\mathbf{k})\rangle.\end{aligned}\tag{F1}$$

If $R^n = E$, then we have

$$\prod_{s=0,\ldots,n-1}\mathcal{B}(R^s\mathbf{k})=\mathcal{I}_{N_{\mathrm{occ}}\times N_{\mathrm{occ}}}.\tag{F2}$$

If $R^n = \bar{E}$, we have

$$\prod_{s=0,\ldots,n-1}\mathcal{B}(R^s\mathbf{k})=(-1)^F\mathcal{I}_{N_{\mathrm{occ}}\times N_{\mathrm{occ}}}.\tag{F3}$$

Now we show that $\mathcal{B}(\mathbf{k})$ is also a unitary matrix:

$$\begin{aligned}[\mathcal{B}(\mathbf{k})\mathcal{B}^\dagger(\mathbf{k})]_{ij}&=\sum_{i'\in\mathrm{occ}}\langle u_i(R\mathbf{k})|\tilde{R}|u_{i'}(\mathbf{k})\rangle\langle u_{i'}(\mathbf{k})|\tilde{R}^\dagger|u_j(R\mathbf{k})\rangle\\&=\langle u_i(R\mathbf{k})|u_j(R\mathbf{k})\rangle\\&=\delta_{ij}.\end{aligned}\tag{F4}$$

In this equation, we have used that the point group operator $\tilde{R}$ is unitary. This is because all symmetry operators are either unitary or antiunitary (Wigner's theorem) and a point group operation does not include either time-reversal or charge conjugation.

Using the sewing matrix, we can represent $|u_i(R\mathbf{k})\rangle$ in terms of $|u_i(\mathbf{k})\rangle$ and the sewing matrix. To see this, first notice that

$$\tilde{R}^{-1}|u_i(R\mathbf{k})\rangle=\sum_{j\in\mathrm{occ}}|u_j(\mathbf{k})\rangle\langle u_j(\mathbf{k})|\mathcal{R}^{-1}|u_i(R\mathbf{k})\rangle,\tag{F5}$$

then multiply $\tilde{R}$ on both sides and obtain

$$|u_i(R\mathbf{k})\rangle=\sum_{j\in\mathrm{occ}}\mathcal{B}^\star_{ij}(\mathbf{k})|u_j(\mathbf{k})\rangle.\tag{F6}$$

Finally, we consider a sewing matrix that is associated with an antiunitary operator $\tilde{R}'$. First we show that the sewing matrix is still unitary:

$$\begin{aligned}&[\mathcal{B}(\mathbf{k})\mathcal{B}^\dagger(\mathbf{k})]_{ij}\\&\quad=\sum_{m\in\mathrm{occ}}\langle u_i(R'\mathbf{k})|\tilde{R}'|u_m(\mathbf{k})\rangle[\langle u_j(R'\mathbf{k})|\tilde{R}'|u_m(\mathbf{k})\rangle]^*.\end{aligned}\tag{F7}$$

Then use the antiunitarity of $\tilde{R}^{-1}$, we have

$$[\langle u_j(R'\mathbf{k})|\hat{R}'u_m(\mathbf{k})\rangle]^*=\langle u_m(\mathbf{k})|\hat{R}'^{-1}|u_j(R'\mathbf{k})\rangle.\tag{F8}$$

And from this, we obtain $\mathcal{B}(\mathbf{k})\mathcal{B}^\dagger(\mathbf{k})=\mathcal{I}_{N_{\mathrm{occ}}\times N_{\mathrm{occ}}}$.

And for an antiunitary operator, we can also express $|u_i(R'\mathbf{k})\rangle$ in terms of $|u_i(\mathbf{k})\rangle$ and the sewing matrix: first notice

$$\hat{R}'^{-1}|u_i(R'\mathbf{k})\rangle=\sum_{j\in\mathrm{occ}}|u_j(\mathbf{k})\rangle\langle u_j(\mathbf{k})|\hat{R}'^{-1}|u_i(R'\mathbf{k})\rangle,\tag{F9}$$

then act $\hat{R}'$ on both sides and have

$$\begin{aligned}|u_i(R\mathbf{k})\rangle&=\sum_{j\in\mathrm{occ}}(\langle u_j(\mathbf{k})|\hat{R}'^{-1}|u_i(R'\mathbf{k})\rangle)^\star\tilde{R}'|u_j(\mathbf{k})\rangle\\&=\sum_{j\in\mathrm{occ}}\langle u_i(R'\mathbf{k})|\hat{R}'|u_j(\mathbf{k})\rangle|u_j(\mathbf{k})\rangle\\&=\sum_{j\in\mathrm{occ}}\mathcal{B}_{ij}|u_j(\mathbf{k})\rangle.\end{aligned}\tag{F10}$$

APPENDIX G: ORBITAL MAGNETOELECTRIC POLARIZATION AND POINT GROUP SYMMETRIES

According to Ref. 38, for a generic tight-binding model the orbital part of the magnetoelectric polarization includes other terms besides the Chern Simon term, given by

$$P^o_{ij}=\frac{e^2}{\hbar}\sum_{n\in\mathrm{occ},m\in\mathrm{occ}}\int_{\mathrm{BZ}}\frac{d^3k}{(2\pi)^3}\mathrm{Re}\left\{\frac{\langle u_n(\mathbf{k})|\partial_i\tilde{P}(\mathbf{k})|u_m(\mathbf{k})\rangle\langle u_m(\mathbf{k})|[\partial\tilde{H}(\mathbf{k})\times\partial\tilde{P}(\mathbf{k})]_j-[\partial\tilde{P}(\mathbf{k})\times\partial\tilde{H}(\mathbf{k})]_j|u_n(\mathbf{k})\rangle}{E_n(\mathbf{k})-E_m(\mathbf{k})}\right\}.\tag{G1}$$

When the insulator has symmetry R (proper or improper), we have

$$\begin{aligned}&\tilde{R}|u_n(\mathbf{k})\rangle=\sum_{n'\in\mathrm{occ}}\mathcal{B}_{n'n}|u_{n'}(R\mathbf{k})\rangle,\quad\tilde{R}|u_m(\mathbf{k})\rangle=\sum_{m'\in\mathrm{unocc}}\bar{\mathcal{B}}_{n'n}|u_{n'}(R\mathbf{k})\rangle,\\&\tilde{R}\tilde{H}(\mathbf{k})\tilde{R}^{-1}=\tilde{H}(R\mathbf{k}),\quad\tilde{R}\tilde{P}(\mathbf{k})\tilde{R}^{-1}=\tilde{P}(R\mathbf{k}),\end{aligned}\tag{G2}$$

where $\bar{\mathcal{B}}(\mathbf{k})$ is the sewing matrix defined for the unoccupied subspace,

$$\bar{\mathcal{B}}_{mn}(\mathbf{k})=\langle u_m(R\mathbf{k})|\tilde{R}|u_n(\mathbf{k})\rangle,\tag{G3}$$

where $m \in$ unocc. Substituting Eq. (G2) into Eq. (G1), we obtain

$$\sum_{n\in\text{occ},m\in\text{unocc}} \frac{\langle u_n(\mathbf{k})|\partial_i \tilde{P}(\mathbf{k})|u_m(\mathbf{k})\rangle\langle u_m(\mathbf{k})|[\partial \tilde{H}(\mathbf{k})\times\partial \tilde{P}(\mathbf{k})]_j|u_n(\mathbf{k})\rangle}{E_n(\mathbf{k})-E_m(\mathbf{k})}$$
$$= \sum_{n,n',n''\in\text{occ},m,m',m''\in\text{unocc}} \mathcal{B}_{nn'}(\mathbf{k})\mathcal{B}^{\dagger}_{n''n}(\mathbf{k})\bar{\mathcal{B}}_{m'm}(\mathbf{k})\bar{\mathcal{B}}^{\dagger}_{mm''}(\mathbf{k})$$
$$\times \frac{\langle u_{n'}(R\mathbf{k})|\partial_i \tilde{P}(R\mathbf{k})|u_{m'}(R\mathbf{k})\rangle\langle u_{m''}(R\mathbf{k})|[\partial \tilde{H}(R\mathbf{k})\times\partial \tilde{P}(R\mathbf{k})]_j|u_{n''}(R\mathbf{k})\rangle}{E_n(\mathbf{k})-E_m(\mathbf{k})}. \tag{G4}$$

Then we use the fact that since $\tilde{R}$ is a symmetry, the energy eigenvalue is unchanged under $\tilde{R}$, i.e., $E_m(\mathbf{k}) = E_{m'}(R\mathbf{k})$ and $E_n(\mathbf{k}) = E_{n'}(R\mathbf{k})$. Therefore the summation over m,n only appears in the numerator, and using the unitarity of $\mathcal{B}(\mathbf{k})$ and $\bar{\mathcal{B}}(\mathbf{k})$, we have

$$\sum_{n\in\text{occ},m\in\text{unocc}} \frac{\langle u_n(\mathbf{k})|\partial_i \tilde{P}(\mathbf{k})|u_m(\mathbf{k})\rangle\langle u_m(\mathbf{k})|[\partial \tilde{H}(\mathbf{k})\times\partial \tilde{P}(\mathbf{k})]_j|u_n(\mathbf{k})\rangle}{E_n(\mathbf{k})-E_m(\mathbf{k})}$$
$$= \sum_{n'\in\text{occ},m'\in\text{unocc}} \frac{\langle u_{n'}(R\mathbf{k})|\partial_i \tilde{P}(R\mathbf{k})|u_{m'}(R\mathbf{k})\rangle\langle u_{m'}(R\mathbf{k})|[\partial \tilde{H}(R\mathbf{k})\times\partial \tilde{P}(R\mathbf{k})]_j|u_{n'}(R\mathbf{k})\rangle}{E_{n'}(R\mathbf{k})-E_{m'}(R\mathbf{k})}. \tag{G5}$$

Define $\partial' = \partial/\partial(R\mathbf{k}) = R^{-1}\partial$, then we have

$$\partial_i \tilde{P} = R_{ii'}\partial'_{i'}\tilde{P}, \quad (\partial\tilde{H}\times\partial\tilde{P})_j = \det(R)R_{jj'}(\partial'\tilde{H}\times\partial'\tilde{P})_{j'}. \tag{G6}$$

Combining Eqs. (G6), (G5), and (G1), we obtain the following simple formula:

$$P^o_{ij} = \det(R)R_{ii'}R_{jj'}P^o_{i'j'}. \tag{G7}$$

From Eq. (G7), we can see that P^o_{ij} transforms like a rank-two tensor except for a factor of $\det(R)$, which is -1 for improper rotations.

From this relation, we can see that PGS in general places constraints on the components of P^o_{ij}. Specially, for space inversion, $R = -I_{3\times3}$ and Eq. (G7) implies that every component must vanish. For mirror reflection about the xy plane, we have $R_{ij} = \delta_{ij}(1-2\delta_{3j})$, and Eq. (G7) gives $P^o_{ii} = P^o_{xy} = 0$, while $P^o_{xz,zx,yz,zy}$ can take nonzero values. For improper rotation S_4, we have $P^o_{xz,yz,zx,zy,zz} = 0$ and $P^o_{xx} = -P^o_{yy}$ and $P^o_{xy} = P^o_{yx}$.

[1] R. B. Laughlin, Phys. Rev. Lett. **50**, 1395 (1983).
[2] X. G. Wen, Adv. Phys. **44**, 405 (1995).
[3] G. Moore and N. Read, Nucl. Phys. B **360**, 362 (1991).
[4] X. L. Qi, Y. S. Wu, and S. C. Zhang, Phys. Rev. B **74**, 085308 (2006).
[5] C. L. Kane and E. J. Mele, Phys. Rev. Lett. **95**, 146802 (2005).
[6] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, Science **314**, 1757 (2006).
[7] L. Fu and C. L. Kane, Phys. Rev. B **74**, 195312 (2006).
[8] L. Fu, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. **98**, 106803 (2007).
[9] J. E. Moore and L. Balents, Phys. Rev. B **75**, 121306 (2007).
[10] M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. Molenkamp, X.-L. Qi, and S.-C. Zhang, Science **318**, 766 (2007).
[11] H. Zhang, C.-X. Liu, X.-L. Qi, X. Dai, Z. Fang, and S.-C. Zhang, Nat. Phys. **5**, 438 (2009).
[12] L. Fu and C. L. Kane, Phys. Rev. Lett. **100**, 096407 (2008).
[13] A. Kitaev, AIP Conf. Proc. **1134**, 10 (2009).
[14] A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, Phys. Rev. B **78**, 195125 (2008).
[15] K. Sun, W. V. Liu, A. Hemmerich, and S. Das Sarma, Nat. Phys. **8**, 67 (2011).
[16] X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Phys. Rev. B **83**, 205101 (2011).
[17] G. Xu, H. Weng, Z. Wang, X. Dai, and Z. Fang, Phys. Rev. Lett. **107**, 186806 (2011).
[18] C. Fang, M. J. Gilbert, X. Dai, and B. A. Bernevig, Phys. Rev. Lett. **108**, 266802 (2012).
[19] G. B. Halász and L. Balents, Phys. Rev. B **85**, 035103 (2012).
[20] K. v. Klitzing, G. Dorda, and M. Pepper, Phys. Rev. Lett. **45**, 494 (1980).
[21] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982).
[22] F. D. M. Haldane, Phys. Rev. Lett. **61**, 2015 (1988).
[23] X.-L. Qi, T. Hughes, and S.-C. Zhang, Phys. Rev. B **78**, 195424 (2008).
[24] X. L. Qi and S. C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011).
[25] X.-L. Qi, T. L. Hughes, and S.-C. Zhang, Phys. Rev. B **78**, 195424 (2008).
[26] D. Hsieh, D. Qian, L. Wray, Y. Xia, Y. S. Hor, R. J. Cava, and M. Z. Hasan, Nature (London) **452**, 970 (2008).
[27] D. Hsieh, Y. Xia, D. Qian, L. Wray, J. H. Dil, F. Meier, L. Patthey, J. Osterwalder, A. Fedorov, A. B. H. Lin, D. Grauer, Y. Hor, R. Cava, and M. Hasan, Nature (London) **460**, 1101 (2009).
[28] D. Hsieh, Y. Xia, L. Wray, D. Qian, A. Pal, J. H. Dil, J. Osterwalder, F. Meier, G. Bihlmayer, C. L. Kane, Y. S. Hor, R. J. Cava, and M. Z. Hasan, Science **323**, 919 (2009).

[29]Q. Liu, C.-X. Liu, C. Xu, X.-L. Qi, and S.-C. Zhang, Phys. Rev. Lett. **102**, 156603 (2009).
[30]X. Zhou, C. Fang, W.-F. Tsai, and J. P. Hu, Phys. Rev. B **80**, 245317 (2009).
[31]L. Fu, Phys. Rev. Lett. **106**, 106802 (2011).
[32]T. L. Hughes, E. Prodan, and B. A. Bernevig, Phys. Rev. B **83**, 245132 (2011).
[33]A. M. Turner, Y. Zhang, R. S. K. Mong, and A. Vishwanath, Phys. Rev. B **85**, 165120 (2012).
[34]L. Fu and C. L. Kane, Phys. Rev. B **76**, 045302 (2007).
[35]T. Hsieh, H. Lin, J. Liu, W. Duan, A. Bansil, and L. Fu, Nat. Commun. **3**, 982 (2012).
[36]A. Alexandradinata, X. Dai, and B. A. Bernevig, arXiv:1208.4234 (2012).
[37]R. Resta, Rev. Mod. Phys. **66**, 899 (1994).
[38]A. M. Essin, A. M. Turner, J. E. Moore, and D. Vanderbilt, Phys. Rev. B **81**, 205104 (2010).
[39]A. Malashevich, I. Souza, S. Coh, and D. Vanderbilt, New J. Phys. **12**, 053032 (2010).
[40]R. Slager, A. Mesaros, V. Juricis, and J. Zaanen (unpublished).