Spin-Orbit-Free Topological Insulators without Time-Reversal Symmetry

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(Received 14 March 2014; published 12 September 2014)

We explore the 32 crystallographic point groups and identify topological phases of matter with robust surface modes. For $n = 3, 4,$ and 6 of the $C_{nv}$ groups, we find the first-known 3D topological insulators without spin-orbit coupling, and with surface modes that are protected only by point groups; i.e., the relevant symmetries are purely crystalline and do not include time reversal. To describe these $C_{nv}$ systems, we introduce the notions of (a) a halved mirror chirality, an integer invariant which characterizes half-mirror-planes in the 3D Brillouin zone, and (b) a bent Chern number, the traditional Thouless–Kohmoto–Nightingale–den Nijs invariant generalized to bent 2D manifolds. We find that a Weyl semimetallic phase intermediates two gapped phases with distinct halved chiralities. In addition to electronic systems without spin-orbit coupling, our findings also apply to intrinsically spinless systems such as photonic crystals and ultracold atoms.

DOI: 10.1103/PhysRevLett.113.116403 PACS numbers: 71.20.-b, 73.20.-r

Insulating phases are deemed distinct if they cannot be connected by continuous changes of the Hamiltonian that preserve both the energy gap and the symmetries of the phase; in this sense we say that the symmetry protects the phase. Distinct phases have strikingly different properties—of experimental interest are the presence of boundary modes, which in many cases distinguish a trivial and a topological phase. The symmetries that are ubiquitous in crystals belong to the space groups, and among them the point groups are the sets of transformations that preserve a spatial point. Despite the large number of space groups in nature, there are few known examples in which boundary modes are protected by crystal symmetries alone [1–4]. In this Letter, we explore the 32 crystallographic point groups and identify topological phases of matter with robust surface modes. For $n = 3, 4,$ and 6 of the $C_{nv}$ groups, we find the first-known 3D topological insulators (TIs) without spin-orbit coupling, and with surface modes that are protected only by point groups; our findings differ from past theoretical proposals [5–7] in not needing time-reversal symmetry (TRS). To describe these $C_{nv}$ systems, we introduce the notions of (a) a halved mirror chirality, an integer invariant which characterizes half-mirror planes in the 3D Brillouin zone, and (b) a bent Chern number, the traditional Thouless–Kohmoto–Nightingale–den Nijs invariant [8] generalized to bent 2D manifolds (illustrated in Fig. 1).

To date, all experimentally realized TIs are strongly spin-orbit coupled, and a variety of exotic phenomenon originate from this coupling, e.g., Rashba spin-momentum locking on the surface of a TI [16]. Considerably less attention has been addressed to spinless systems, i.e., insulators and semimetals in which spin-orbit coupling is negligibly weak [4,5]. The topological classifications of spinless and spin-orbit-coupled systems generically differ. A case in point is SnTe, a prototypical $C_{nv}$ system with strong spin-orbit coupling [2,17]. In SnTe, the mirror Chern number [1] was introduced to characterize planes in the 3D BZ which are invariant under reflection, or mirror planes in short. The Bloch wave functions in each mirror plane may be decomposed according to their representations under reflection, and each subspace may exhibit a quantum

![FIG. 1 (color online). Bottom: (a) Half-mirror-planes (HMPs) in the 3D Brillouin zone (BZ) of a hexagonal lattice with $C_{6h}$ symmetry. Blue face that projects to $\bar{K} - K$: HMP$_1$. Brown, $K - K'$: HMP$_2$. Red, $\bar{K} - K'$: HMP$_3$. (b) HMPs in the 3D BZ of a tetragonal lattice with $C_{4h}$ symmetry. Red face that projects to $\bar{K} - M$: HMP$_4$. Blue, $\bar{K} - \bar{X} - M$: HMP$_5$. (c) Blue face that projects to $\bar{K} - K$: HMP$_6$. Note that the black-colored submanifold in (c) is not a HMP. In each of (a),(b) and (c) we define a bent Chern number on the triangular pipe with its ends identified. Top: Nonblack lines are half-mirror lines (HMLs) in the corresponding 2D BZ of the 001 surface; each HML connects two distinct $C_n$-invariant points with $n \ge 2$.](image-url)
always trivial due to twofold rotational symmetry and if the point group satisfies the following criterion: there surface modes can exist without mirror Chern numbers, which is fulfilled by crystals with representations (irreps) of the little group at each surface BZ, which admit two-dimensional irreducible characterizations orbitals that transform in the 2D irrep of the reflection operator. On these HMLs, we would like to translations by a reciprocal lattice vector. (b) All Bloch points are mapped to itself under an doublet irreps, and all other irreps are of the singlet kind. However, for \( n \) e.g., (C\(_{3v}\)), there are two independent mirror Chern numbers, defined as \( C_e \left( C_o \right) \) in the mirror-even (odd) subspace [9]. In both (a) and (b), \( C_e \) and \( C_o \) are defined on a single mirror plane indicated in red; in (b), the two red lines correspond to two projected planes which connect through a reciprocal lattice vector (dashed arrow).

In this work, we propose that point-group-protected surface modes can exist without mirror Chern numbers, if the point group satisfies the following criterion: there exist at least two high-symmetry points \((k_1, k_2)\) in the surface BZ, which admit two-dimensional irreducible representations (irreps) of the little group [19] at each point. This is fulfilled by crystals with \( C_{4v} \) and \( C_{6v} \) symmetries, but not \( C_{2v} \). There exist in nature two kinds of \( C_{3v} : C_{3v}^{(a)} \) and \( C_{3v}^{(b)} \), which differ in the orientation of their mirror planes; compare Fig. 2(a) with Fig. 2(b). Only \( C_{3v}^{(b)} \) fulfills our criterion. Henceforth, \( C_{nv} \) is understood to mean \( C_{4v} \), \( C_{4v} \), and \( C_{6v} \). We are proposing that surface bands of \( C_{nv} \) systems assume topologically distinct structures on lines which connect \( k_1 \) to \( k_2 \). We are particularly interested in half-mirror lines (HMLs), that each satisfies two conditions. (a) It connects two distinct \( C_{nv} \)-invariant points for \( m > 2 \); we illustrate this in Fig. 1, where a \( C_{nv} \)-invariant point is mapped to itself under an \( m \)-fold rotation, up to translations by a reciprocal lattice vector. (b) All Bloch wave functions in a HML may be diagonalized by a single reflection operator. On these HMLs, we would like to characterize orbitals that transform in the 2D irrep of \( C_{nv} \), e.g., \((p_x, p_y)\) or \((d_{xz}, d_{yz})\) orbitals. We refer to these as the doublet irreps, and all other irreps are of the singlet kind.

We begin by parametrizing HML\(_i\) with \( s_i \in [0, 1] \), where \( s_i = 0 \) (1) at the first (second) \( C_{nv} \)-invariant point. The subscript \( i \) labels the different HMLs in a \( C_{nv} \) system, the \( i \)th HML is invariant under a specific reflection \( M_i \). At \( s_i = 0 \) and 1, (001) surface bands form doubly degenerate pairs with opposite mirror eigenvalues, irrespective of whether the system has TRS. To prove this, let \( U(g) \) represent the symmetry element \( g \) in the orbital basis. Suppose \( U(M_i) |\eta\rangle = |\eta\rangle \) for \( \eta \in \{\pm 1\} \). By assumption, \( |\eta\rangle \) transforms in the doublet representation; i.e., it is a linear combination of states with complex eigenvalues \( \eta \). The degeneracies at momenta \( s = 0 \) and \( s = 1 \) are as dispersing linearly with momentum. This is true if the little group of the wave vector \( \pm s \in \{0, 1\} \) is \( C_{3v} \), but for \( C_{4v} \) and \( C_{6v} \) such crossings are in reality quadratic [9].

![FIG. 2 (color online).](image)

(a) Top-down view of hexagonal BZ with \( C_{3v}^{(a)} \) symmetry; our line of site is parallel to the rotational axis. (b) Hexagonal BZ with \( C_{3v}^{(b)} \) symmetry. (c) Tetragonal BZ with \( C_{4v} \) symmetry. (d) Hexagonal BZ with \( C_{6v} \) symmetry. Reflection-invariant planes are indicated by solid lines. Except the line through \( \Gamma \), all nonequivalent \( C_{nv} \)-invariant lines are indicated by circles for \( n = 2 \), triangles for \( n = 3 \), and squares for \( n = 4 \). For each of \( \{C_{3v}^{(a)}, C_{3v}^{(b)}\} \), there are two independent mirror Chern numbers, defined as \( C_e \left( C_o \right) \) in the mirror-even (odd) subspace [9]. In both (a) and (b), \( C_e \) and \( C_o \) are defined on a single mirror plane indicated in red; in (b), the two red lines correspond to two projected planes which connect through a reciprocal lattice vector (dashed arrow).

![FIG. 3 (color online).](image)

Distinct connectivities of the (001) surface bands along the half-mirror lines. Black solid (dotted) lines indicate surface bands with eigenvalue \( +1 \) (\(-1\)) under reflection \( M_i \); crossings between solid and dotted lines are robust due to reflection symmetry. For simplicity, we have depicted all degeneracies at momenta \( s = 0 \) and \( s = 1 \) as dispersing linearly with momentum. This is true if the little group of the wave vector \( \pm s \in \{0, 1\} \) is \( C_{3v} \), but for \( C_{4v} \) and \( C_{6v} \) such crossings are in reality quadratic [9].
For spinless representations, $M^2 = I$, and we label bands with mirror eigenvalue $+1$ ($-1$) as mirror-even (mirror-odd). $F_e$ ($F_o$) is defined as the Berry curvature of occupied doublet bands [20,21], as contributed by the mirror-even (-odd) subspace.

For $C^{(b)}_{3v}$, there exists three independent HMPs as illustrated in Fig. 1(a), which we label by $i \in \{1, 2, 3\}$; all other HMPs are related to these three by symmetry. The $C_{6v}$ group is obtained from $C^{(b)}_{3v}$ by adding sixfold rotational symmetry, which enforces $\chi_2 = 0$, and $\chi_1 = -\chi_3$. The sign in the last identity is fixed by our parametrization of $\{t_i\}$, which increase in the directions indicated by blue arrows in Fig. 2. Thus, HMP$_1$ is the sole independent HMP for $C_{6v}$. Finally, we find that there are two HMPs for $C_{4v}$, labeled by $i \in \{4, 5\}$ [Fig. 1(b)]. Unlike the other highlighted HMPs, $C_{4v}$ is the union of two mirror faces, HMP$_{4a}$ and HMP$_{5b}$, which are related by a $\pi/2$ rotation. States in HMP$_{3b}$ are invariant under the reflection $M_y : y \rightarrow -y$, while in HMP$_{5b}$ the relevant reflection is $M_x : x \rightarrow -x$. The product of these orthogonal reflections is a $\pi$ rotation ($C_2$) about $z$, thus $M_y = C_2 M_y$. In the doublet representation, all orbitals are odd under a $\pi$ rotation, thus $U(C_2) = -I$ and all states in HMP$_3$ may be labeled by a single operator $M_y \equiv M_5$.

The invariants $\{\chi_i\}$ are well defined so long as bulk states in the HMPs are gapped, which is true of $C_{nv}$ insulators. These invariants may also be used to characterize $C_{nv}$ semimetals, so long as the gap closes away from the HMPs. Such band touchings are generically Weyl nodes [22,23], though exceptions exist with a conjunction of time-reversal and inversion symmetries [24]. The chirality of each Weyl node is its Berry charge, which is positive (negative) if the node is a source (sink) of Berry flux. By the Nielsen-Ninomiya theorem, the net chirality of all Weyl nodes in the BZ is zero [25]. To make progress, we divide the BZ into “unit cells,” such that the properties of one unit cell determine all others by symmetry. As seen in Fig. 1, these unit cells resemble the interior of triangular pipes; they are known as the orbifolds $T^3/C_{nv}$. The net chirality of an orbifold can be nonzero, and is determined by the Chern number on the 2D boundary of the orbifold. As each boundary resembles the surface of a triangular pipe, we call it a bent Chern number. We define $C_{123}$, $C_{45}$, and $C_6$ as bent Chern numbers for $C^{(b)}_{3v}$, $C_{4v}$, and $C_{6v}$, respectively. $C^{(b)}_{3v}$ systems in the doublet representation are described by four invariants $(\chi_1, \chi_2, \chi_3, C_{123})$, which are related by parity $|\chi_1 + \chi_2 + \chi_3| = \text{parity}[C_{123}]$ [9]. If $\sum_{i=1}^3 \chi_i$ is odd, $C_{123}$ must be nonzero due to an odd number of Weyl nodes within the orbifold, which implies the system is gapless. If the system is gapped, $\sum_{i=1}^3 \chi_i$ must be even. However, the converse is not implied. For $C_{4v}$, a similar relation holds: parity $|\chi_4 + \chi_5| = \text{parity}[C_{4v}]$ [9]. These parity constraints may be understood in light of a Weyl semimetallic phase that intermediates two gapped phases with distinct halved chiralities. There are four types of events that alter the halved chirality $\chi_i$ of HMP$_i$: we explain how Weyl nodes naturally emerge in the process. (i) Suppose the gap closes between two mirror-even bands in HMP$_i$. Around this band touching, bands disperse linearly within the mirror plane, and quadratically in the direction orthogonal to the plane. Within HMP$_i$, the linearized Hamiltonian around the band crossing describes a massless Dirac fermion in the even representation of reflection. If the mass of the fermion inverts sign, $\int_{\text{HMP}_i} \mathcal{F}_e / 2\pi$ changes by $\eta \in \{\pm 1\}$, implying that $\chi_i$ also changes by $\eta$ through (1). This quantized addition of Berry flux is explained by a splitting of the band touching into two Weyl nodes of opposite chirality, and on opposite sides of the mirror face [Fig. 4(a)]. In analogy with magnetostatics, the initial band touching describes the nucleation of a dipole, which eventually splits into two opposite-charge monopoles; the flux through a plane separating two monopoles is unity. (ii) The same argument applies to the splitting of dipoles in the mirror-odd subspace, which alters $\int_{\text{HMP}_i} \mathcal{F}_o / 2\pi$ by $\kappa \in \{\pm 1\}$, and $\chi_i$ by $-\kappa$. For (iii) and (iv), consider two opposite-charge monopoles which converge on HMP$_i$ and annihilate, causing $\chi_i$ to change by unity. The sign of this change...
is determined by whether the annihilation occurs in the mirror-even or -odd subspace. As modeled in the Supplemental Material [9], the transition between two distinct gapped phases is characterized by a transfer of Berry charge between two distinct HMPs [Figs. 4(e)–4(g)]. In the intermediate semimetallic phase, the experimental implications include Fermi arcs on the (001) surface [23,26,27].

We hope our classification stimulates a search for materials with \( \text{C}_{nv} \) symmetry. Why is \( \text{C}_{nv} \) special? We propose sufficient criteria for gapless surface modes whose robustness rely on a symmetry group. Minimally, (i) the symmetry must be unbroken by the presence of the surface. Additionally, either (ii) a reflection symmetry exists so that mirror subspaces can display a quantum anomalous Hall effect, or (iii) there exist at least two high-symmetry points in the surface BZ, which admit higher-than-one-dimensional irreps of the symmetry group. In addition to predicting new topological materials, these criteria are also satisfied by the well-known SnTe class, [2] and also the \( \mathbb{Z}_2 \) insulators [6,7,28–35]. Among the 32 crystallographic point groups, only the \( \text{C}_n \) and \( \text{C}_{nv} \) groups are preserved for a surface that is orthogonal to the rotational axis [19].

Though all \( \text{C}_{nv} \) groups satisfy (ii), the lack of spin-orbit coupling implies only \( \text{C}_{3v}^{(a)} \) and \( \text{C}_{3v}^{(b)} \) systems can have nonvanishing mirror Chern numbers [9]. While all \( \text{C}_n \) groups by themselves only have one-dimensional irreps, the \( \text{C}_4 \) or \( \text{C}_6 \) group satisfies (iii) in combination with TRS, as is known for the topological crystalline insulators introduced in Ref. [5]. Finally, only a subset of the \( \text{C}_{nv} \) groups possess two-dimensional irreps which satisfy (iii): \( \text{C}_{3v}^{(a)}, \text{C}_{4v}, \) and \( \text{C}_{6v} \). In the second row of Table I, we list the topological invariants which characterize \( \text{C}_{3v}, \text{C}_{4v}, \) and \( \text{C}_{6v} \), for bands of any irrep. In addition to the well-known mirror Chern numbers \( (\text{C}_4, \text{C}_6) \), we have introduced the bent Chern numbers as a measure of the Berry charge in each orbifold \( T^3/\text{C}_{nv} \). If the orbital character of bands near the gap is dominated by the doublet irreps, then the halved mirror chirality \( \chi_i \) becomes a useful characterization, as seen in the third row of Table I. In particular, the mirror Chern numbers of \( \text{C}_{3v}^{(b)} \) are completely determined by \( (\chi_1, \chi_2, \chi_3, \chi_{123}) \) [9]. The singlet and doublet irreps of realistic systems are often hybridized. The topological surface bands that we predict here are robust, so long as this hybridization does not close the bulk gap, and if there are no errant singlet surface bands within the gap [5].

We discuss generalizations of our findings. In addition to materials whose full group is \( \text{C}_{nv} \), we are also interested in higher-symmetry materials whose point groups reduce to \( \text{C}_{nv} \) subgroups in the presence of a surface, for \( n = 3, 4, \) or 6. We insist that these higher-symmetry point groups have neither (a) a reflection plane that is orthogonal to the principal \( \text{C}_n \) axis, nor (b) a twofold axis that lies perpendicular to the \( \text{C}_n \) axis, and parallel to the mirror plane. The presence of either (a) or (b) imposes \( \chi = \text{C}_n = \text{C}_o = 0 \) in any (half) mirror-plane of the \( \text{C}_{nv} \) system [9].

Only one such higher-symmetry point group exists: \( D_{3d} \) reduces to \( \text{C}_{3v} \) on the 111 surface [10]. Many \( \text{C}_{nv} \) systems naturally have TRS, which constrains all \( \text{C}_{3v}^{(a)} \) and \( \text{C}_{3v}^{(b)} \) invariants in Table I to vanish, with one independent exception for \( \text{C}_{3v}^{(b)}; \chi_1 = -\chi_3 \) can be nonzero [9]. TRS does not constrain the invariants of \( \text{C}_{4v} \) or \( \text{C}_{6v} \). Our analysis of charge-conserving systems are readily generalized to spinless superconductors which are describable by mean-field theory. Because of the particle-hole redundancy of the mean-field Hamiltonian, the only nonvanishing invariants from Table I belong to \( \text{C}_{3v}^{(a)} \) and \( \text{C}_{3v}^{(b)} \), among these nonvanishing invariants, the only constraint is \( \chi_1 = \chi_3 \) for \( \text{C}_{3v}^{(b)} \) [9]. While we have confined our description to electronic systems without spin-orbit coupling, the halved chirality is generalizable to photonic crystals which are inherently spinless, and also to cold atoms. Finally, we point out that the bent Chern number and the halved chirality are also valid characterizations of spin-orbit-coupled systems with mirror symmetry. In particular, (1) applies to representations with spin if we redefine the mirror-even (odd) bands as having mirror eigenvalues \( +i \) (\( -i \)) [9]. The implications are left to future work.

A.A. is grateful to Yang-Le Wu and Tim Lou for insightful interpretations of this work. A. A. and B. A. B. were supported by the Packard Foundation, 339-4063–Keck Foundation, NSF CAREER DMR-095242, ONR-N00014-11-1-0635, and NSF-MRSEC DMR-0819860 at Princeton University. This work was also supported by DARPA under SPAWAR Grant No. N66001-11-1-4110. C. F. is supported by ONR-N0014-11-1-0728 and DARPA-N66001-11-1-4110. M. J. G. acknowledges support from the ONR under Grants No. N0014-11-1-0728 and No. N0014-14-1-0123, and the Center for Advanced Study (CAS) at the University of Illinois.

TABLE I. Topological classification of spinless insulators and semimetals with \( \text{C}_{nv} \) symmetry.

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