Local and global topology for $Z_2$ Dirac points

Tiantian Zhang,1,2, * Daisuke Hara,1 and Shuichi Murakami1,2,†

1Department of Physics, Tokyo Institute of Technology, Ookayama, Meguro-ku, Tokyo 152-8551, Japan
2Tokodai Institute for Element Strategy, Tokyo Institute of Technology, Nagatsuta, Midori-ku, Yokohama, Kanagawa 226-8503, Japan

Symmetries are always entangled with topology. In systems with time-reversal ($\mathcal{T}$) and glide ($\mathcal{G}$) symmetries, $Z_2$ monopole charge $\mathcal{Q}$ defined by the time-reversal-glide symmetry $\tilde{\Theta} = \mathcal{T}\mathcal{G}$ for Dirac points is considered to accompany double/quadr-helicoid surface states (DHSSs/QHSSs) in previous studies. Here we study the topology of $\mathcal{Q}$ for $Z_2$ Dirac points and establish its bulk-surface correspondence with strict proofs. By improving the previous gauge-dependent definition of $\mathcal{Q}$, we find that $\mathcal{Q}$ is equivalent to the $\mathcal{G}$-invariant $\nu$ mathematically and physically in $Z_2$-Dirac systems. This result is counterintuitive, since $\nu$ is always trivial in $\mathcal{T}$-preserving gapped systems, and was thought to be ill-defined in gapless systems. We give a gauge-invariant formula for $\mathcal{Q}$, which is associated with DHSSs in both the spinless and spinful systems with single $\mathcal{G}$. $\mathcal{Q}$ is formulated in a simpler form in spinless systems with two vertical $\mathcal{G}$, associated with QHSSs, which is also entangled with filling-enforced topological band insulators in some space groups. Since $\mathcal{Q}$ is ill-defined in spinful systems with two vertical $\mathcal{G}$, QHSSs will not be held. The first material candidate Li$_2$B$_4$O$_7$ together with a list of possible space groups preserving QHSSs are also proposed for demonstration on our theory and further studies.

Starting from the first proposal of the $\mathcal{T}$-protected topological insulator in 2005 [1–3], a vast number of topological (crystalline) insulators were discovered in gapped band structures with different symmetries afterwards [4–10]. Topological equivalence of two systems can be diagnosed by either the type or the value of topological invariants, which are global quantum numbers defined uniquely with different symmetries and associated with diverse topological surface states due to bulk-surface correspondence. For example, a $Z_2$ type topological invariant $\nu$ is proposed in $\mathcal{T}$-breaking gapped systems with $\mathcal{G}$-symmetry [11, 12], where the topological crystalline insulator (TCI) phase can be obtained when $\nu = 1$, associated with a single unpinned surface Dirac cone located along $\mathcal{G}$-invariant lines. Particularly, for $\mathcal{T}$-breaking spinless systems with two vertical $\mathcal{G}$, another $Z_2$ type topological invariant, i.e., symmetry-based indicator $\mu_2$, is offered to diagnose the $\mathcal{G}$-protected TCI phase [13], which was conjectured to be associated with the filling-enforced band insulators in some cases.

Along with the topological investigations in band insulators is the emergence of the topological semimetals, where the band touching points are protected by various topological invariants associated with disparate bulk-surface correspondence. Such as the Berry phase $\gamma$ for the nodal line/ring with drumhead surface states [14–18], the $Z$ type monopole charge $\mathcal{C}$ for Weyl points with helical surface states [19–28] and $Z_2$ type monopole charge $\mathcal{Q}$ for Dirac points with double (quad-)helicoid surface states (DHSSs/QHSSs) [12, 23, 29–33]. In particular, DHSSs/QHSSs associated with $Z_2$ Dirac points realized in $\mathcal{T}$- and $\mathcal{G}$-preserving systems are particularly interesting due to their intriguing shapes, yet their topological nature has not been understood so far. Notably, the bulk-surface correspondence for the $Z_2$ Dirac points is just taken for granted in the previous studies without strict proofs. Furthermore, the known definition of the $Z_2$ monopole charge $\mathcal{Q}$ is not gauge invariant, and thus is insufficient for discussing topological properties. Last but not least, topological invariants like $\nu$ and $\mu_2$ have been studied only for gapped $\mathcal{G}$-preserving systems, and there is no research studying their relationships with $\mathcal{Q}$ so far. Thus, a thorough and comprehensive study on $Z_2$ Dirac points carrying monopole charge $\mathcal{Q}$ is increasingly recognized as serious concerns in the recent studies [23, 32, 33].

In this work, we start the discussion for conventional Dirac points composed of two Weyl points with opposite $\mathcal{C}$ in $\mathcal{T}$- and $\mathcal{G}$-preserving systems, and then discuss $Z_2$ Dirac points carrying monopole charge $\mathcal{Q}$ protected by $\tilde{\Theta}$. We list several main results that are innovative and even counterintuitive: (i) The $Z_2$ monopole charge $\mathcal{Q}$ is redefined to ensure gauge invariance, leading to an easily evaluated formula, which implies a global nature of $\mathcal{Q}$; (ii) We extended the definition of the $\mathcal{G}$-protected global topological invariant $\nu$ to the gapless systems with Dirac points. $\nu$ was thought to be well-defined only in gapped systems, and it vanishes when $\mathcal{T}$ is present. But we find $\nu$ can be nontrivial and equal to $\mathcal{Q}$ in gapless systems with $\mathcal{T}$; (iii) We establish bulk-surface correspondence for $Z_2$ Dirac points with DHSSs for $\mathcal{T}$-preserving systems with one $\mathcal{G}$ both in spinless and spinful systems; (iv) We establish bulk-surface correspondence for $Z_2$ Dirac points with QHSSs for $\mathcal{T}$-preserving systems with two vertical $\mathcal{G}$. It can be only retained in spinless systems, and it vanish in spinful systems due to the ill-defined $\mathcal{Q}$; (v) The first $Z_2$ Dirac material candidate Li$_2$B$_4$O$_7$ and a list of space groups with QHSSs will be offered.

* zhang.t.ac@m.titech.ac.jp
† murakami@stat.phys.titech.ac.jp
$Z$ type and $Z_2$ type monopole charges for Weyl and Dirac points

As a local topological invariant for a Weyl point, the monopole charge $C$ can be defined by the Chern number on a sphere enclosing the Weyl point, or on a two-dimensional (2D) plane in the 3D Brillouin zone (BZ) marked by the dashed line in Fig. 1 (a1). The former definition shows the local property of $C$, while the latter one offers a global point of view to understand the influence of $C$ to the rest part of the BZ, which gives rise to gapless surface states connecting two Weyl points with opposite monopole charges, as shown in Fig. 1 (a3). Fermi arcs are isoenergetic surface states, and they can disappear when those two Weyl points are projected onto the same momentum on the surface BZ or when they are forced to coalesce into a Dirac point by additional symmetries [34–43], as shown in Figs. 1 (a1–a2), where the purple solid line is the Fermi arc. Although the monopole charge $C$ will vanish for a pair of Weyl points or a Dirac point [29, 36, 44–46], a new local $Z_2$ topological invariant $Q$ can be defined when an anti-unitary operator $\tilde{\Theta}$ with $\tilde{\Theta}^2 = -1$ is present [23], and its corresponding topological bulk degeneracies are named $Z_2$ Weyl dipoles or $Z_2$ Dirac points. Due to the restriction of Nielson-Ninomiya theorem, $Z_2$ Dirac points and Weyl dipoles always appear in pairs and are located at $T$-related momenta in the BZ. Since $Z_2$ Weyl dipoles and $Z_2$ Dirac points can be transformed mutually by $\tilde{\Theta}$-preserved perturbations, we will use $Z_2$ Dirac points as an example to show the local and global topology of $Q$ in the following.

$Z_2$ Monopole charge $Q$ with one glide symmetry

We consider systems with one glide symmetry $G_y = \{M_y|_{\frac{1}{2}00}\}$. Let $\tilde{\Theta}_y$ denote an antiunitary operator $\tilde{\Theta}_y = T G_y$, which leads to $\tilde{\Theta}_y^2 = e^{-i k_x \gamma_y}$. Therefore $k_x = \pi$ is a special plane where $\tilde{\Theta}_y^2 = -1$ is satisfied, and here we consider the case with two $Z_2$ Dirac points (Weyl dipoles) on the $k_x = \pi$ plane in the 3D BZ. They are related by $T$ symmetry (see Fig. 1 (b1)), and so they cannot appear at time-reversal-invariant momenta (TRIM). Thus, $Z_2$ Dirac points are usually located on high-symmetry lines for systems only has one $G$, and at non-TRIM high-symmetry points for systems with two vertical $G$.

Analogous to $C$, the $Z_2$ monopole charge $Q$ is defined in terms of wavefunctions on a sphere enclosing the Dirac point [23]. But distinctively, we notice that it is in fact determined by wavefunctions on a circle on the $\tilde{\Theta}_y^2 = -1$ plane ($k_z = \pi$) enclosing the Dirac point, and it is not gauge invariant. To make it well-defined and gauge invariant, we need to fix the gauge, so that the circle can be enlarged to the rectangle $R$ shown in Fig. 1 (b1) without obstruction (See the Supplementary Material Sec. S2 for details). It is possible only when the bulk band structure on the $k_z = \pi$ is gapped except for the Dirac points.

FIG. 1. Fermi arcs and surface-state connections for Weyl points and Dirac points. (a1) Fermi arcs for Weyl points with opposite monopole charges $C$, which can be defined either by the sphere enclosed the Weyl point or by a 2-dimensional plane marked by the dashed line. (a2) Fermi arcs do not necessarily exist for a conventional Dirac point composed of a pair of Weyl points with opposite $C$. (a3) Helical surface states for a pair of Weyl points carrying opposite $C$. (b1) Locations for $Z_2$ Dirac points (Weyl dipoles) on the $k_x = \pi$ plane (blue plane) satisfying $\tilde{\Theta}_y^2 = -1$ in the bulk BZ. (b2) Double-helicoid surface states contributed by $Z_2$ Dirac points, which will be projected along $M$-$X$ on the surface BZ. The gray cone is the bulk $Z_2$ Dirac band. Blue and yellow sheets are the anticrossing helical surface states. Purple lines show the surface-state connections along $\Gamma$-$X$-$M$ directions. (b3) Fermi arcs for $Z_2$ Dirac points (Weyl dipoles) on the $G_y$-preserved surface BZ, which corresponds the gray plane shown in (b1). The Fermi arcs will rotate to (b4) when the energy changes. (b5-b6) Two possible surface-state connections along $\Gamma$-$X$-$M$ directions. (b7) Fermi arcs for $Z_2$ Dirac points (Weyl dipoles) on the $G_y$-preserved surface BZ, which corresponds the gray plane shown in (b1). The Fermi arcs will rotate to (b4) when the energy changes. (b5-b6) Two possible surface-state connections along $\Gamma$-$X$-$M$ directions. (b7-b8) Two possible topological surface-state connections for $Z_2$ Dirac points in the spinless and $T$-preserving case. (b9-b10) Two possible topological surface-state connections for $Z_2$ Dirac points in the spinful and $T$-preserving case. Surface states shown in (b7-b10) are all in the double-helicoid shape shown in (b2).
considered. In the end, $Q$ is equal to the difference of $\Theta$-polarization $P_{\Theta}$, calculated by the Berry phase along the two blue lines shown in Fig. 1 (b1):

$$Q = P_{\Theta}(k_y = \pi) - P_{\Theta}(k_y = 0) \quad (\text{mod } 2), \quad (1)$$

where $P_{\Theta}(k_y) = \frac{1}{\pi L} (\gamma_L^+ + \gamma_L^-)$, $\gamma_L$ is the Berry phase with the integral path $L$ taken as $k_y = 0$ and $k_y = \pi$ lines (blue lines in Fig. 1 (b1)) on the $k_x = \pi$ plane and “±” represent the sectors with positive or negative glide eigenvalues for the Bloch wavefunctions. We call $P_{\Theta}(k_y)$ $\Theta$-polarization because $\Theta_y$ switches those two glide sectors. Thus, although $Q$ is a local topological invariant, it also has a global nature due to the definition in Eq. (1).

We further notice from Eq. (1) that $Q$ is equal to the global $G$-protected $Z_2$ topological invariant $\nu$ mathematically and physically in both the spinless and spinful systems (Supplementary Material Sec. S1 and S2 for details):

$$Q = \nu. \quad (2)$$

This is counterintuitive since $\nu$ is defined for fully gapped systems and it vanishes when the system is $T$-invariant \cite{11, 12}, while $Q$ is associated with the Dirac point in $T$-preserving gapless systems. We propose in this paper that $\nu$ is also well-defined by Eq. (1), even for gapless systems, as long as the system is fully gapped along the two blue lines marked in Fig. 1 (b1). It is nontrivial when the system is $T$-invariant and have Dirac cones on the $M-X$ line. The nontrivial $Q (= \nu)$ results in topological surface states on the $G_y$-preserving (001) surface, with the shape of the double helicoid (Fig. 1 (b2)), which will be shown in detail in the next section.

**Bulk-surface correspondence for $Q$ with one glide symmetry** Observing topological states on the surface is the simplest and most straightforward way to demonstrate the topology of the bulk states, due to the bulk-surface correspondence. Here we establish bulk-surface correspondence for a nonzero $Q$ with one $G$ symmetry in both the spinless and spinful cases with $T$ symmetry. In the present case, two Dirac points are projected onto the $M-X$ line satisfying $\Theta_y^2 = -1$. The Fermi energy is set at the Dirac point. As we show in the following, the Fermi arcs for a nonzero $Q$ have two possibilities shown in Figs. 1 (b3-b4) on the $G_y$-preserving surface BZ, where the surface states extend either toward $M$ or $X$. The green dashed lines are glide-invariant ones, and the green solid lines are $\Theta_y$-invariant ones, with $\Theta_y^2 = -1$, giving rise to double degeneracy for surface states.

In gapped systems with $G_y$ symmetry, the bulk $Z_2$ topological invariant $\nu_y$ is well-defined, and by the bulk-surface correspondence, it is equal to the surface $Z_2$ topological invariant $\nu_{y, \text{surface}}$ which characterizes how the surface states cross the Fermi energy (see Supplementary Material Sec. S3 for details). However, in the present gapless system, $\nu_y$ remains well-defined by Eq. (1), while
$\nu_{\text{surface}}$ becomes ill-defined due to the bulk gap closing along $\tilde{M}-\tilde{X}$. To establish bulk-surface correspondence for $T$-preserving gapless systems with $\nu_y = 1$, firstly, we slightly break the $T$ symmetry to open a small bulk gap at the Dirac point. Figures 1 (b5-b6) are two possible nontrivial surface-state connections in gapped band structures without $T$, which has a single unpinched surface Dirac cone along the glide-invariant lines, $\tilde{M}-\tilde{Y}-\tilde{M}'$ or $\tilde{X}-\Gamma-\tilde{X}'$, but not both, corresponding to $\nu_{\text{surface}}=1$. Next, we make the $T$-breaking perturbation to be zero: all the states along $\tilde{X}-\tilde{M}$ then becomes doubly degenerate due to $\Theta^2 = -1$. Through this procedure, we find that two different kinds of nontrivial surface-state connections are possible, both without SOC (Figs. 1 (b7-b8)) and with SOC (Figs. 1 (b9-b10)). The corresponding Fermi arcs are shown in Figs. 1 (b3-b4). Remarkably, the doubly degenerate surface states should start exactly at the Dirac point, belonging to the DHSSs shown in Fig. 1 (b2). These DHSSs can be interpreted as a superposition of surface states from two Weyl points with opposite $\mathcal{C}$, and their intersections are protected along $\tilde{X}-\tilde{M}$ by $\Theta^2 = -1$, in both the spinless and spinful systems. Such DHSSs also have a $Z_2$ nature, which directly follows from the $Z_2$ nature of $\nu$ in gapped systems [11, 12]. For example, when there are two Dirac points within $0 < k_y < \pi$ on the $k_z = \pi$ plane, two sets of DHSSs are expected, but they can be annihilated by a continuous change of surface states without changing the bulk bands.

In Ref. [23], it is proposed that crossing of the surface states, if any, will not be avoided along the $\tilde{M}-\tilde{X}$ with $\Theta^2 = -1$, allowing the DHSSs. Nonetheless, this does not necessarily guarantee existence of the DHSSs. Our theory has established the bulk-surface correspondence for $Z_2$ Dirac points, guaranteeing appearance of the DHSSs.

In [47], the surface-state connections for topological (crystalline) insulators are classified based on wallpaper groups for $T$-preserving gapped systems with SOC. Such classification cannot be applied to gapless systems focused in this paper. Indeed, while the surface-state connections for spinful gapped systems with $T$ and $\mathcal{G}$ symmetries are always topologically trivial (see Supplementary Materials Sec. S3 for details), those for gapless systems can be nontrivial ($\nu_y = 1$) (see Figs. 1(b7)-(b10)).

**Monopole charge $Q$ with two vertical glide symmetries in spinless systems** $Z_2$ Dirac systems with two $\Theta$ have more unresolved mysteries, and we find that $Q$ is well-defined only in the spinless systems, which is beyond people’s expectation [23]. In the presence of two vertical glide symmetries, such as $\mathcal{G}_x = \{M_x, |0\bar{2}0\}$ and $\mathcal{G}_y = \{M_y, |1\bar{4}0\}$ in #110, those two vertical glide symmetries lead to $\Theta^2_x = -1$ at $k_x = \pi$ and $\Theta^2_y = -1$ at $k_y = \pi$, resulting in $Z_2$ Dirac points at non-TRIM high-symmetry points, e.g., $P$ and $P'$.

The original formula for the $Z_2$ glide invariant $\nu$ is expressed as a sum of integrals in $k$-space, but it can be expressed in terms of irreducible representations in the presence of other symmetries [48, 49]. Since two vertical $\mathcal{G}_x$ and $\mathcal{G}_y$ will give rise to an additional $C_{2z}$ symmetry in spinless systems, the formula of $\nu(=Q)$ can be simplified into that in terms of the $C_{2z}$ eigenvalues, which will be explained with space group #110 (see the Supplementary Material Sec. S4 for details):

$$(-1)^\nu = \prod_i \frac{C_i(G)}{C_i(X)}, \quad (3)$$

where $C_i$ is the eigenvalue of $C_{2z}$ for the $i^{th}$ occupied band. $G$ and $X$ are two $C_{2z}$-invariant high-symmetry momenta on the $k_z = 0$ plane, which are labelled in Fig. 3 (b). We note that there are two inequivalent $X$ points for #110, but we do not need to distinguish them in Eq. (3) because they are on the same $C_{2z}$ axis due to the non-primitive nature of the lattice. Therefore, we get $\nu_x = \nu_y$, and simply write $\nu$ in Eq. (3). In the present case, $\nu$ in Eq. (1) is ill-defined because the presence of the bulk Dirac point on the blue lines in Fig. 1 (b1), but instead, we can use Eq. (3) to safely define $\nu$. Equation (3) is a new formula for $Q(=\nu)$ calculated by the symmetry data at TRIM, and in fact, since the $Z_2$ Dirac points are located at non-TRIM, it is also equal to the symmetry-based indicator $\mu_2$ proposed for spinless gapped systems with two vertical $\mathcal{G}$, when a $T$-breaking perturbation is introduced to open a gap for the Dirac points [13]:

$$\mu_2 = \sum_{\mathbf{k}: \text{TRIM at } k_z=0} \frac{n_+^k - n_-^k}{4} \equiv -(n^-_\Gamma + n^-_X) \pmod{2}, \quad (4)$$

where $n^\pm_k$ is the number of occupied eigenstates with the positive and negative eigenvalue for $C_{2z}$ at $k$ (\in TRIM). $\mu_2$ is also entangled with filling-enforced band insulators when there is full gap of the system, because $\mu_2$ is related to the filling $N$ by $\mu_2 \equiv (N/2 \pmod{2})$ in the space group #110. Therefore, insulators with $N = 4m + 2$ (mod 2) ($m$: integers) are nontrivial in #110 [49].

**Bulk-surface correspondence for $Q$ with two vertical glide symmetries in spinless systems** By combining our results on systems with one $\mathcal{G}$, we show bulk-surface correspondence for $T$-preserving systems with two vertical $\mathcal{G}$.

Figure 2 (a) shows the surface BZ on (001) surface preserving two vertical $\mathcal{G}$. In $T$-preserving spinless systems with two vertical $\mathcal{G}$, $Z_2$ Dirac points are projected to $\tilde{M}$ on the (001) surface BZ, which makes $\nu_{\text{surface}}$ and $\nu_{\text{surface}}$ well-defined and defined to be equal to $\nu_x(=\nu_y)$, which will give rise to two possible nontrivial surface-state connections with a single surface Dirac cone pinned at $X$ and $Y$, respectively, as summarized in Figs. 2 (c-d). Next, when the $T$ symmetry is restored, doubly degenerate surface states along the surface BZ boundaries protected by $\Theta^2 = -1$ will appear. The corresponding surface-state connections for QHSSs along high-symmetry lines are shown in Figs. 2 (e) and (f).

Here, doubly degenerate surface states start exactly from the Dirac point at $\tilde{M}$ and connect either to $\tilde{X}$ or
to \( \bar{Y} \) with the protection of \( \Theta^2 = -1 \) or \( \tilde{\Theta}^2 = -1 \) along the BZ boundaries. Away from the \( M - \bar{X} \) or \( M' - \bar{Y} \) line, this degeneracy will be split toward the conduction and valence bands, showing the QHSSs with two quantum spin Hall (QSH) like flows along \( Y - \bar{\Gamma} - X \) directions, as marked by the purple lines in Fig. 2 (h). This conclusion is supported by our tight-binding model calculation for \#110 shown in Fig. 2 (g), where the purple and blue lines represent the surface states obtained from the top and bottom of the slab (See the Supplementary Material Sec. S6 for details). The surface-state filling at \( X/M \) and \( X'/M' \) will be changed by one when the surface states cross through the \( Z_2 \) Dirac points, showing the helicoid nature of the surface states.

In spinful systems with two vertical \( G \), \( Q \) for the bulk Dirac point is ill-defined because of the presence of other bulk degeneracies at TRIM on the \( \bar{\Theta}^2 = -1 \) planes, in contrast to spinless systems. Therefore, the bulk-surface correspondence will also be eliminated. Correspondingly, the surface states are not of a quad-helicoid shape. Since \( \bar{M} \) is invariant under \( G_x \) and \( T \), fourfold degenerate surface states consisting of \( \phi \), \( G_x \phi \), \( T \phi \) and \( TG_x \phi \) (\( \phi \): an eigenstate of \( G_x \)) appear. The surface states around \( \bar{M} \) are formed by two surface Dirac cones with twofold degeneracies along the surface BZ boundaries, which is quite similar with the ones for wallpaper group of \( \bar{p}2gg \) on the \((001)\) surface with two vertical glide mirror symmetries, and surface with \( \bar{p}4gg \) is forbidden to have QHSSs.

**\( Z_2 \) Dirac material Li\(_2\)B\(_4\)O\(_7\) with QHSSs** QHSSs are the consequence of bulk-surface correspondence for \( Z_2 \) Dirac points with two vertical \( G \), as well as the bridge for connecting \( Q \), \( \nu \) and \( \mu_2 \). Thus, discovering materials with QHSSs will not only offer platforms to verify our theory, but also be essential for a wide range of further experimental and theoretical studies. Although Eq. (3) for \( Z_2 \) Dirac points with two vertical \( G \) is derived from \#110, it still holds for other space groups that we list in Tab. I with proper high-symmetry momenta (details are in the supplementary Sec. S5). Among those 6 space groups, only \#73, \#110 and \#142 can be converted to filling-enforced band insulators with filling \( N = 4m + 2 \) when \( T \)-breaking perturbations are introduced.

By following Tab. I, we propose the first experimentally synthesized material candidate Li\(_2\)B\(_4\)O\(_7\) with \#110 [50] and two \( Z_2 \) Dirac fermions in its spinless electronic band structure. As shown in Figs. 3 (a-c), all the fourfold band crossings at \( P \) and \( P' \) are \( Z_2 \) Dirac points, which will be projected onto the corner point \( M \) on \((001)\) surface. Figure 3 (e) is the surface state calculation on \((001)\) surface, following the \( k \)-path marked in Fig. 3 (f). Two groups of anticrossing helical surface states with different Fermi velocity (chirality) together with degenerate surface states along surface BZ boundaries show the QHSSs feature of Li\(_2\)B\(_4\)O\(_7\).

QHSSs can be also obtained in systems with \( Z_2 \) Weyl dipoles. After breaking \( C_{4z} \) symmetry, the symmetry of Li\(_2\)B\(_4\)O\(_7\) is lowered to \#45 and two \( Z_2 \) Dirac points split into two pairs of \( Z_2 \) Weyl dipoles along \( k_z \) direction, i.e., \( W_1 + W_2 \) and \( W'_1 + W'_2 \), respectively, as shown in Figs. 3 (h) and (d). Since \( \bar{\Theta} \) and \( \bar{\Theta}_y \) are still preserved in \#45, each pair of Weyl dipole will also carry a nonzero \( Q \) and leads to QHSSs on the \((001)\) surface, as shown in Figs. 3 (g) and (h), which are quite similar with the ones from two \( Z_2 \) Dirac points. Within a pair of the Weyl dipole, \( W_1 \) and \( W_2 \) cannot be annihilated with each other due to the nonzero \( Q \), although their total monopole charge \( C \) is zero, which is different from general Weyl semimetals. (More materials with QHSSs contributed by Weyl dipoles are in the supplementary Sec. S7)

**Conclusion** We offer a full understanding on the topology of \( T \bar{G} \)-protected \( Z_2 \) Dirac points in this paper. We redefined the \( Z_2 \) monopole charge \( Q \) protected by \( (T \bar{G})^2 = -1 \) to meet the gauge-invariant condition, and find \( Q \) is equal to \( \bar{G} \)-protected topological invariant \( \nu \) in \( Z_2 \) Dirac systems. \( Q \) can be formulated into a simpler form in terms of irreducible representations at two TRIM when two vertical \( G \) are present. We study the bulk-surface correspondence in spinless and spinful systems with one \( G \) associated with DHSSs, and in spinless systems with two vertical \( G \) associated with QHSSs. Bulk-surface correspondence for spinful systems with two vertical \( G \) will vanish due to the ill-defined \( Q \) of the system. Since QHSSs in spinless \( Z_2 \) Dirac systems with two vertical symmetries is the bridge to unify \( Q \), \( \nu \), symmetry-based indicator \( \mu_2 \) and even filling-enforced band insulators, we offer the first material example Li\(_2\)B\(_4\)O\(_7\) and a list of space groups which may obtain QHSSs for further exploration.

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| Space group | Two vertical glide mirrors | Location | Momenta used for Eq. (3) |
|-------------|--------------------------|----------|------------------------|
| #73         | \( \{M_x \mid \bar{z}, \bar{x}, 0\} \); \( \{M_y \mid \bar{z}, 0, 0\} \) | W        |\( \Gamma, T \) |
| #110        | \( \{M_x \mid \bar{z}, \bar{x}, 0\} \); \( \{M_y \mid \bar{z}, \bar{x}, 0\} \) | P        |\( \Gamma, X \) |
| #142        | \( \{M_x \mid \bar{z}, \bar{x}, 0\} \); \( \{M_y \mid \bar{z}, \bar{x}, 0\} \) | P        |\( \Gamma, X \) |
| #206        | \( \{M_x \mid \bar{z}, \bar{x}, 0\} \); \( \{M_y \mid \bar{z}, \bar{x}, 0\} \) | P        |\( \Gamma, N \) |
| #228        | \( \{M_x \mid \bar{z}, \bar{x}, 0\} \); \( \{M_y \mid \bar{z}, \bar{x}, 0\} \) | W        |\( \Gamma, X \) |
| #230        | \( \{M_x \mid \bar{z}, \bar{x}, 0\} \); \( \{M_y \mid \bar{z}, \bar{x}, 0\} \) | P        |\( \Gamma, N \) |

**TABLE I.** Spinless systems where \( Z_2 \) Dirac points associated with QHSSs may be obtained. Each column represents for the space group number, two vertical glide mirrors which protect the \( Z_2 \) Dirac points together with \( T \), the momentum where \( Z_2 \) Dirac points are located and the momenta used for Eq. (3). We note that all the space groups listed here have a wallpaper group of \( p2gg \) on the \((001)\) surface with two vertical glide mirror symmetries, and surface with \( \bar{p}4gg \) is forbidden to have QHSSs.
FIG. 3. Quad-helicoid surface states in Li$_2$B$_2$O$_7$. (a) Crystal structure and band structure for Li$_2$B$_2$O$_7$. (b) BZ and surface BZ for both #110 and #45 along [001] direction. (c-d) spinless band structure of Li$_2$B$_2$O$_7$ for #110 and #45, respectively. (e-f) and (g-h) are QHSSs calculated on the (001) surface for #110 and #45, respectively, where the $k$ paths are followed by the ones marked in (f) and (h). (f) and (h) are the Fermi arcs calculated around two $Z_2$ Dirac points located at $M$, with the energy contour marked by the black dashed line in (e) and (g), respectively.
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