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Z_2 topology in nonsymmorphic crystalline insulators: Möbius twist in surface states

Ken Shiozaki,[1] Masatoshi Sato,[2] and Kiyonori Gomi[3]
[1]*Department of Physics, Kyoto University, Kyoto 606-8502, Japan*
[2]*Department of Applied Physics, Nagoya University, Nagoya 464-8603, Japan*
[3]*Department of Mathematical Sciences, Shinshu University, Nagano 390-8621, Japan*
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It has been known that an antiunitary symmetry such as time-reversal or charge conjugation is needed to realize $\mathbf{Z}_2$ topological phases in noninteracting systems. Topological insulators and superconducting nanowires are representative examples of such $\mathbf{Z}_2$ topological matters. Here we report the $\mathbf{Z}_2$ topological phase protected by only unitary symmetries. We show that the presence of a nonsymmorphic space group symmetry opens a possibility to realize $\mathbf{Z}_2$ topological phases without assuming any antiunitary symmetry. The $\mathbf{Z}_2$ topological phases are constructed in various dimensions, which are closely related to each other by Hamiltonian mapping. In two and three dimensions, the $\mathbf{Z}_2$ phases have a surface consistent with the nonsymmorphic space group symmetry, and thus they support topological gapless surface states. Remarkably, the surface states have a unique energy dispersion with the Möbius twist, which identifies the $\mathbf{Z}_2$ phases experimentally. We also provide the relevant structure in the K theory.

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I. INTRODUCTION

Symmetry is a key for recent developments on topological phases. For instance, time-reversal symmetry and its resultant Kramers degeneracy are essential for the stability of quantum spin Hall states [1,2] and three-dimensional (3D) topological insulators [3–5]. Also, the particle-hole symmetry (or charge conjugation symmetry) in superconductors makes it possible to realize topological superconductors [6–18] which support exotic Majorana fermions on their boundary. Based on these symmetries, many candidate systems for topological insulators and superconductors have been proposed theoretically and examined experimentally [19–24].

In addition to the general symmetries of time reversal and charge conjugation, materials have their own symmetry specific to the structures. In particular, crystals are invariant under space group symmetry, like inversion, reflection, discrete rotation, and so on. Such crystalline symmetries also provide a new class of topological phases, which are dubbed topological crystalline insulators [25,26] and topological crystalline superconductors [27–30]. Surface states protected by crystalline symmetry have been confirmed experimentally [31–33]. Furthermore, a systematic classification of such topological phases and topological defects has been done theoretically [34–36].

In the study of topological crystalline insulators and superconductors, much attention has been paid to those protected by point group symmetries [37–39]. However, point groups are not the only allowed crystalline symmetries. Space groups contain a transformation which is not a simple point group operation but a combination of a point group operation and a nonprimitive lattice transformation. This class of transformations is called nonsymmorphic. Despite that many crystals have such nonsymmorphic symmetries, only a few have been known for their influence on topological phases [40,41].

In this paper, we show that the presence of nonsymmorphic space group symmetries provides unique $\mathbf{Z}_2$ topological phases: Being different from other known $\mathbf{Z}_2$ phases, the new $\mathbf{Z}_2$ phases need no antiunitary symmetry like time reversal or charge conjugation. We present the $\mathbf{Z}_2$ topological phases in various dimensions, which are closely related to each other. In two and three dimensions, the $\mathbf{Z}_2$ phases may have a surface consistent with the nonsymmorphic space group symmetry, and thus they support topological gapless surface states. Unlike helical surface Dirac modes in other $\mathbf{Z}_2$ phases, the surface states have a peculiar energy dispersion with Möbius twist, which provides a distinct experimental signal for these phases. The $\mathbf{Z}_2$ topological stability of the surface states and a relevant structure in the K theory are also discussed.

II. NONSYMMORPHIC CHIRAL SYMMETRY IN ONE DIMENSION

As the simplest example, we first consider a one-dimensional (1D) system. In one dimension, no nonsymmorphic operation is consistent with the existence of a boundary, and thus no boundary zero energy state is topologically protected by this symmetry. Nevertheless, we can show that an interesting nontrivial $\mathbf{Z}_2$ bulk topological structure appears by a nonsymmorphic unitary symmetry. The 1D system is also useful to construct $\mathbf{Z}_2$ nontrivial topological phases in higher dimensions, which have gapless boundary states protected by nonsymmorphic symmetries.

The symmetry we consider is a nonsymmorphic version of the chiral symmetry: Instead of the ordinary chiral symmetry,

$$\{\Gamma, H_{1\mathrm{D}}(k_x)\} = 0, \quad \Gamma^2 = 1, \tag{1}$$

where Γ is given by a k_x-independent unitary matrix, we consider a k_x-dependent chiral symmetry with

$$\{\Gamma_{1\mathrm{D}}(k_x), H_{1\mathrm{D}}(k_x)\} = 0, \quad \Gamma_{1\mathrm{D}}^2(k_x) = e^{-ik_x}. \tag{2}$$

By imposing 2π periodicity in k_x on $\Gamma(k_x)$, the simplest $\Gamma_{1\mathrm{D}}(k_x)$ is

$$\Gamma_{1\mathrm{D}}(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}, \tag{3}$$

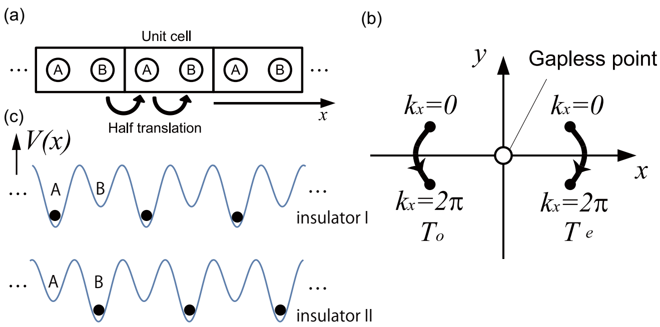

FIG. 1. (Color online) (a) Two inequivalent sites A and B in the unit cell. (b)Topologically different trajectories $(x(k_x),y(k_x))$. (c) Insulating states I (top) and II (bottom).

where $\Gamma_{\rm 1D}(k_x)$ acts on two inequivalent sites A and B in the unit cell. As illustrated in Fig. 1(a), $\Gamma_{\rm 1D}(k_x)$ exchanges these two sites, followed by a *half translation* in the lattice space.

The Hamiltonian with the nonsymmorphic chiral symmetry has a generic form

$$H_{\rm 1D}(k_x)=\begin{pmatrix} x(k_x) & -iy(k_x)e^{-ik_x/2} \\ iy(k_x)e^{ik_x/2} & -x(k_x)\end{pmatrix}, \tag{4}$$

with real functions $x(k_x)$ and $y(k_x)$. The 2π periodicity of the Hamiltonian, $H_{\rm 1D}(k_x+2\pi)=H_{\rm 1D}(k_x)$, implies

$$x(k_x+2\pi)=x(k_x),\quad y(k_x+2\pi)=-y(k_x). \tag{5}$$

Because the eigenvalues of the Hamiltonian are $E(k_x)=\pm\sqrt{[x(k_x)]^2+[y(k_x)]^2}$, the system is gapped at $E=0$ unless the vector $(x(k_x),y(k_x))$ passes through the origin (0,0) at some k_x.

Now we will show that the Hamiltonian (4) has two distinct topological phases: As we show in Fig. 1(b), the Hamiltonian defines a trajectory of $(x(k_x),y(k_x))$ in the xy plane, when k_x changes from 0 to 2π. From the constraint of Eq. (5), the trajectory forms an open arc, not a closed circle, and the end point $(x(2\pi),y(2\pi))$ must be the mirror image of the start point $(x(0),y(0))$ with respect to the x axis. The open trajectory passes the x axis an odd number of times. More precisely, we have two different ways to cross the x axis; if the trajectory passes the positive x axis an odd (even) number of times, then it must pass the negative x axis an even (odd) number of times. See trajectories $\rm T_o$ and $\rm T_e$ in Fig. 1(c). These two different trajectories cannot be continuously deformed into each other without gap closing, since the gap of the system closes if they go across the origin. Therefore, by counting the parity of times the trajectory passes the negative x axis, we can identify the two distinct phases of the Hamiltonian (4). The $\boldsymbol{Z}_2$ nature of the topological phase is discussed in detail in the Appendix.

If the parity is odd (even), then the Hamiltonian is adiabatically deformed into the k_x-independent Hamiltonian $H_{\rm o}$ ($H_{\rm e}$) in the below, without gap closing,

$$H_{\rm o}=-\sigma_z,\quad H_{\rm e}=\sigma_z, \tag{6}$$

with the Pauli matrix σ_i $[i=0,x,y,z]$. These Hamiltonians suggest a simple physical realization of the nonsymmorphic chiral symmetry. Consider a periodic potential with two different local minima A and B in the unit cell [see Fig. 1(c)]. If the energy of the local minimum A (B) is much higher than B's (A's) and tunnelings between local minima are neglected, we have an insulating phase I (II) in the half filling, for which an effective Hamiltonian is given by $H_{\rm e}$ ($H_{\rm o}$). Our argument above implies that these insulating phases are topologically distinct and they are separated by a topological quantum phase transition as long as one keeps the symmetry (2). Such a periodic system could be artificially created by cold atoms.

III. NONSYMMORPHIC Z_2 SYMMETRY IN TWO DIMENSIONS

Much more interesting $\boldsymbol{Z}_2$ topological phases protected by nonsymmorphic symmetries appear in two and three dimensions. In these dimensions, a class of nonsymmorphic symmetries are consistent with the presence of a surface, and thus the symmetry protected gapless edge states may appear. Here we present a two-dimensional (2D) $\boldsymbol{Z}_2$-topological nonsymmorphic insulator, which supports a unique edge state.

To obtain the $\boldsymbol{Z}_2$ phase, we use a Hamiltonian map that increases the dimension of the system. This map keeps the topological structure by shifting symmetries, and is known to be useful to classify the topological (or topological crystalline) insulators/superconductors [36,42]. In particular, the periodic structure of the topological table is explained by this map. The details of the map in the present case and the relevant structure in the K theory are given in the Appendix.

From the Hamiltonian mapping, we obtain a representative Hamiltonian of a 2D $\boldsymbol{Z}_2$ topological nonsymmorphic insulator,

$$H_{\rm 2D}(k_x,k_y)=(m+\cos k_y)\tau_y\otimes H_{\rm 1D}(k_x)+\sin k_y\tau_x\otimes\sigma_0, \tag{7}$$

which has a k_x-dependent nonsymmorphic symmetry

$$[U(k_x),H_{\rm 2D}(k_x,k_y)]=0,\quad U(k_x)=\tau_x\otimes\Gamma_{\rm 1D}(k_x), \tag{8}$$

and the additional chiral symmetry,

$$\{\Gamma,H_{\rm 2D}(k_x,k_y)\}=0,\quad \Gamma=\tau_z\otimes\sigma_0, \tag{9}$$

where τ_i $(i=0,1,2,3)$ is the Pauli matrix for the degrees of freedom on which Γ acts. These two symmetry operators anticommute:

$$\{\Gamma,U_{\rm 2D}(k_x)\}=0. \tag{10}$$

Here note that the nonsymmorphic symmetry $U_{\rm 2D}(k_x)$ commutes with $H_{\rm 2D}(k_x,k_y)$, although it is constructed from $\Gamma_{\rm 1D}(k_x)$ anticommuting with $H_{\rm 1D}(k_x)$. Whereas any terms consistent with the symmetries (8) and (9) can be added to the Hamiltonian, the basic topological properties can be captured by Eq. (7). For a gapped $H_{\rm 1D}(k_x)$, the system has a gap unless $m=\pm1$. Using the symmetries (8) and (9), we can define a $\boldsymbol{Z}_2$ invariant, which is nontrivial (trivial) if $-1<m<1$ ($m>1$ or $m<-1$) (see Appendix). Without loss of generality, we assume in the following that the parity of $H_{\rm 1D}(k_x)$ is even, so it is topologically equivalent to $H_{\rm e}=\sigma_z$.

If we consider a boundary parallel to the x axis, we can keep the symmetries (8) and (9). This boundary supports gapless edge states when the system is topological ($-1<m<1$): To demonstrate this, consider a semi-infinite system ($y>0$) with the edge at $y=0$. Since $H_{\rm 1D}(k_x)$ is topologically equivalent to σ_z, we first consider the spatial case of the Hamiltonian (7) with $H_{1D}(k_x) = \sigma_z$. In this particular case, the Hamiltonian $H_{2D}(k_x,k_y)$ does not depend on k_x, and thus the topological edge state should be a k_x-independent zero energy state. The edge state can be obtained analytically when the system is close to the topological phase transition at $m = \pm 1$. Near the topological phase transition, say at $m = -1$, the low energy physics is well described by the effective Hamiltonian obtained by the expansion of Eq. (7) around $k_y = 0$. Then, replacing k_y with $-i\partial_y$, we have the equation for the edge state,

$$\left[\left(m + 1 + \partial_y^2/2\right)\tau_y \otimes \sigma_z - i\partial_y \tau_x \otimes \sigma_0\right]\psi(y) = 0, \quad (11)$$

with the boundary condition $\psi(0) = 0$ and $\psi(\infty) = 0$. If the system is in the topological side near the transition, i.e., $\delta m \equiv m + 1 > 0$, the equation has two independent solutions localized at $y = 0$:

$$\begin{aligned} |\psi_1\rangle &= \begin{pmatrix}1\\0\end{pmatrix}_\tau \otimes \begin{pmatrix}0\\1\end{pmatrix}_\sigma e^{-y}\sinh(\sqrt{-2\delta m + 1}\,y),\\ |\psi_2\rangle &= \begin{pmatrix}0\\1\end{pmatrix}_\tau \otimes \begin{pmatrix}1\\0\end{pmatrix}_\sigma e^{-y}\sinh(\sqrt{-2\delta m + 1}\,y). \end{aligned} \quad (12)$$

On the other hand, in the nontopological side ($\delta m < 0$), the solutions diverge, and the edge states disappear. A similar result is found near another transition point at $m = 1$. We have also confirmed numerically the existence of the zero energy edge mode for the whole region of $-1 < m < 1$.

For a general k_x-dependent $H_{1D}(k_x)$, the zero energy edge states have a k_x-dependent energy dispersion. By diagonalizing the mixing matrix $\langle\psi_i|(\delta m + \partial_y^2/2)\tau_y \otimes (H_{1D}(k_x) - \sigma_z)|\psi_j\rangle$, the energy is evaluated as $E(k_y) \propto \pm y(k_x)$. Then, from the constraint (5), there must be an odd number of zeros for $y(k_x)$ in $k_x \in [0,2\pi]$, and thus the energy dispersion becomes helical $E(k_y) \sim \pm c(k_x - k_0)$ around each zero k_0, as illustrated in Fig. 2(a).

Since the Hamiltonian $H_{2D}(k_x,k_y)$ commutes with $U(k_x)$, the helical dispersion is decomposed into chiral and antichiral ones, each of which is an eigenstate of $U(k_x)$. These two chiral dispersions are mapped to each other by the chiral symmetry Γ, because Γ maps a gapless state to another one, reversing the slope of the dispersion. Furthermore, they belong to different eigensectors of $U(k_x)$, because Γ exchanges the eigenvalues of $U(k_x)$ due to $\{\Gamma, U(k_x)\} = 0$. Therefore, these two chiral dispersions stay gapless without mixing, as far as the symmetries (8) and (9) are retained.

Whereas the above edge state has a similarity to helical edge modes in quantum spin Hall states, their overall structure in the momentum space is completely different: As seen in Fig. 2(a), the present edge state has a unique energy dispersion with the Möbius twist, which is never seen in other $\boldsymbol{Z}_2$ phases. This twist occurs due to the multivaluedness of the eigenvalues $u = \pm e^{-ik_x/2}$ of $U(k_x)$: When one goes round in the k_x direction as $k_x \to k_x + 2\pi$, u changes the sign, so a chiral dispersion in an eigensector of $U(k_x)$ turns smoothly into to an antichiral one in another eigensector.

Another remarkable feature of our edge state is that the constituent chiral dispersions can exchange their eigensectors of $U(k_x)$, as illustrated in Fig. 2(b). This means that any pair of helical dispersions is topologically unstable: When a pair of helical dispersions exists, we can always realize the situation where a chiral dispersion coexists with an antichiral one in the same eigensector of $U(k_x)$, by exchanging the eigensectors properly. Thus, we can open a gap of helical dispersion by mixing between the chiral and antichiral ones.

The arguments above clearly indicate that helical edge states in this system have a $\boldsymbol{Z}_2$ stability like helical edge states in quantum spin Hall systems, although no time-reversal symmetry is required and the mechanism of the stability is completely different from that in quantum spin Hall states.

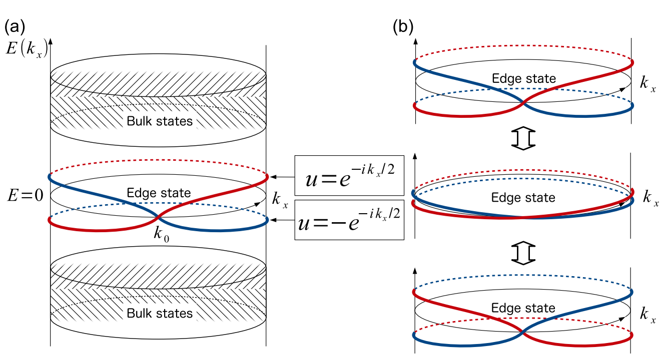

FIG. 2. (Color online) Schematic illustration of edge states with Möbius twist. (a) The red (blue) line is an edge state in the eigensector of $U(k_x)$ with the eigenvalue $u = e^{-ik_x/2}$ ($u = -e^{-ik_x/2}$). (b) An exchange process of the eigensectors, which is carried out by changing the sign of $y(k_x)$ in $H_{1D}(k_x)$ of Eq. (7).

IV. GLIDE REFLECTION SYMMETRY IN 3D

Finally, we consider the system with glide reflection symmetry,

$$\begin{aligned} &G(k_x)H_{3D}(k_x,k_y,k_z)G^{-1}(k_x) = H_{3D}(k_x,k_y,-k_z),\\ &G^2(k_x) = e^{-ik_x}. \end{aligned} \quad (13)$$

The glide reflection $G(k_x)$ is the combination of reflection with respect to the xy plane and translation along the x axis by a half of the lattice spacing. Since $G^2(k_x)$ results in a translation by a unit lattice spacing in the x direction, it provides the nontrivial e^{-ik_x} factor. The $\boldsymbol{Z}_2$ invariant defined by the glide reflection symmetry is given in the Appendix.

A representative Hamiltonian with glide reflection symmetry is given by

$$\begin{aligned} H_{3D}(\boldsymbol{k}) = {}& (m + \cos k_z + \cos k_y)\tau_y \otimes H_{1D}(k_x)\\ &+ \sin k_y \tau_x \otimes \sigma_0 + \sin k_z \tau_z \otimes \sigma_0, \\ G(k_x) = {}& \tau_x \otimes \Gamma_{1D}(k_x). \end{aligned} \quad (14)$$

The 3D system is gapped unless $m = \pm 2, 0$. The $\boldsymbol{Z}_2$ invariant is nontrivial (trivial) when $-2 < m < 0$ or $0 < m < 2$ ($m < -2$ or $m > 2$) (see Appendix).

A surface perpendicular to the y axis retains the glide reflection symmetry, so it may support a gapless surface state protected by this symmetry. For instance, consider a semi-infinite 3D system ($y > 0$) with a surface at $y = 0$, which preserves the glide reflection symmetry. In a manner similar to the 2D system, for the special but topologically equivalent case with $H_{1D}(k_x) = \sigma_z$, we can obtain the surface state analytically near the topological phase transition at $m = \pm 2$: For $m \sim -2$,

$H_{3D}(\boldsymbol{k})$ is well approximated by

$$\hat{H}_{3D} = \left(m + \cos k_z + 1 - \partial_y^2/2\right)\tau_y \otimes \sigma_z - i\partial_y \tau_x \otimes \sigma_0 + \sin k_z \tau_z \otimes \sigma_0. \quad (15)$$

We find that $|\psi_1\rangle$ and $|\psi_2\rangle$ in Eq. (12) with $\delta m = m + \cos k_z + 1$ satisfy the Schrödinger equation,

$$\hat{H}_{3D}\psi_i(y) = E_i(k_z)\psi_i(y), \quad (16)$$

with $E_1(k_z) = \sin k_z$ and $E_2(k_z) = -\sin k_z$, respectively. When the system is in the topological side near the transition, i.e., $-2 < m < 0$, δm is positive (negative) at $k_z = 0$ ($k_z = \pi$). Thus, they meet the boundary condition $\psi_i(0) = 0$ and $\psi_i(\infty) = 0$ near $k_z = 0$, while they diverge near $k_z = \pi$. This means that they form surface states with the linear dispersion $E(k_z) = \pm k_z$ near $k_z = 0$, which merge into bulk states near $k_z = \pi$. On the other hand, in the topologically trivial side, i.e., $m < -2$, δm is always negative, so $|\psi_1\rangle$ and $|\psi_2\rangle$ are no longer physical states anymore. A similar analysis works for $0 < m < 2$, although the surface states appear near $k_z = \pi$ in this case.

For a general $H_{1D}(k_x)$, the surface states have a dispersion in the k_x direction, as well as in the k_z direction: Like the 2D case, the two surface modes, $|\psi_1\rangle$ and $|\psi_2\rangle$, are mixed. The spectrum of the surface states becomes $E(k_x,k_z) = \pm\sqrt{cy^2(k_x) + \sin^2 k_z}$ (c is a constant). From the constraint (5), $y(k_x)$ has an odd number of zeros, and thus the surface states have the corresponding odd number of Dirac cones in the spectrum, as illustrated in Fig. 3.

In the glide invariant plane at $k_z = \Lambda$ ($\Lambda = 0,\pi$) in the Brillouin zone, the Dirac cone has helical dispersions $E \sim \pm c(k_x - k_0)$ in the k_x direction. Since $H_{3D}(\boldsymbol{k})$ commutes with $G(k_x)$ at $k_z = \Lambda$, the helical dispersion can be divided into two eigensectors of $G(k_x)$, which have chiral dispersion and antichiral dispersion, respectively. These two chiral dispersions cannot mix, so a single Dirac cone is topologically stable. On the other hand, a pair of Dirac cones is topologically unstable: From a process similar to Fig. 2(b), the eigensectors can exchange without gap closing. Therefore, from a similar argument in the 2D case, helical dispersions for a pair of Dirac cones can be gapped.

As in the 2D case, the obtained surface state has the following remarkable features: In the k_x direction, which is the direction of the translation for the glide, the surface state has an energy dispersion with the Möbius twist. Furthermore, along the same direction, the surface state is detached from the bulk spectrum. [By adiabatically changing $H_{1D}(k_x)$ as $H_{1D} = \sigma_z$, the surface state becomes even completely flat at $E = 0$ in the k_x direction.] The latter feature in the spectrum can be detected by angle-resolved photoemission. The detachable surface state is never seen in other $\boldsymbol{Z}_2$ phases such as topological insulators. Indeed, any stable Dirac mode in topological insulators bridges the bulk conduction and valence bands in any direction in the surface Brillouin zone. Therefore, this feature provides distinct evidence of this novel $\boldsymbol{Z}_2$ phase.

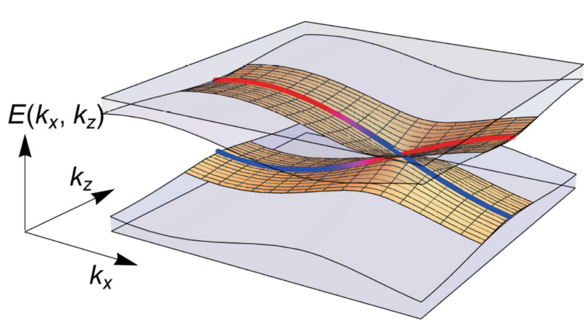

FIG. 3. (Color online) A surface state protected by glide reflection symmetry. The spectrum at $k_z = \Lambda$ has a Möbius twist in the k_x direction: Along the k_x direction, the red branch with the eigenvalue $e^{ik_x/2}$ of $G(k_x)$ turns into the blue one with the eigenvalue $-e^{ik_x/2}$.

A variety of crystal structures like the rutile and diamond ones have glide symmetry. Our consideration here implies that such crystal structures allow an unidentified topological gapless state on a surface keeping the glide symmetry.

We would like to end this section with a remark on an earlier work. It was pointed out in Ref. [40] that there exists a topological phase protected by coexisting mirror reflection and glide symmetries. Despite that a $\boldsymbol{Z}_2$ invariant is introduced in Ref. [40], this phase is essentially a $\boldsymbol{Z}$ phase since the mirror Chern number at a Brillouin zone boundary ($k_z = \pi$) can characterize it as well. In this paper, we extend this result for systems without mirror reflection symmetry by using a different topological argument and a different $\boldsymbol{Z}_2$ invarinat.

V. SUMMARY

We have revealed that nonsymmorphic crystalline symmetries such as glide reflection symmetry provide a class of novel $\boldsymbol{Z}_2$ phases. They are related to each other by Hamiltonian mapping, which is justified by the K theory. These $\boldsymbol{Z}_2$ phases predict remarkable surface states that have the Möbius twist in the spectrum, which can be detectable experimentally.

Note added. Recently, there appeared a complementary and independent work [43] which also discusses a glide protected topological phase.

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APPENDIX

1. Hamiltonian mapping

Here we introduce a Hamiltonian mapping which relates topological phase in different dimensions. A similar map has been used in the classification of topological insulators and superconductors defined on a sphere $\boldsymbol{k} \in S^d$ in the momentum space [36,42]. We generalize the idea to insulators with nonsymmorphic symmetries.

First we review the Hamiltonian mapping used in topological insulators and superconductors. The map is given as follows: If a Hamiltonian $H(\boldsymbol{k})$ on a d-dimensional sphere $\boldsymbol{k} \in S^d$ has chiral symmetry, $\{\Gamma, H(\boldsymbol{k})\} = 0$, with the chiral operator Γ, then the map is

$$H(\boldsymbol{k},\theta) = \sin\theta H(\boldsymbol{k}) + \cos\theta\Gamma, \quad \theta \in [0,\pi], \quad (A1)$$

and if not, it is

$$H(\boldsymbol{k},\theta) = \sin\theta\tau_y \otimes H(\boldsymbol{k}) + \cos\theta\tau_x \otimes \mathbf{1}, \quad \theta \in [0,\pi], \tag{A2}$$

where $\mathbf{1}$ is the unit matrix with the same dimension as $H(\boldsymbol{k})$. Since the mapped Hamiltonian $H(\boldsymbol{k},\theta)$ is independent of $\boldsymbol{k} \in S^d$ at $\theta = 0$ and π, the base space $(\boldsymbol{k},\theta) \in S^d \times [0,\pi]$ of $H(\boldsymbol{k},\theta)$ can be regarded as a $(d+1)$-dimensional sphere S^{d+1} by shrinking S^d to a point at $\theta = 0$ and π, respectively. Thus the mapped Hamiltonian $H(\boldsymbol{k},\theta)$ is defined on S^{d+1}. Furthermore, it can be shown that the map is isomorphic and thus the original $H(\boldsymbol{k})$ and the mapped $H(\boldsymbol{k},\theta)$ have the same topological structures. This map relates topological insulators in different dimensions, and it enables us to study their topological phases systematically.

Using the above isomorphic map, we can construct the 2D insulator

$$H_{2\mathrm{D}}(k_x,k_y) = (m + \cos k_y)\tau_y \otimes H_{1\mathrm{D}}(k_x) + \sin k_y \tau_x \otimes \sigma_0, \tag{A3}$$

with symmetries

$$[U(k_x), H_{2\mathrm{D}}(k_x,k_y)] = 0, \quad U(k_x) = \tau_x \otimes \Gamma_{1\mathrm{D}}(k_x),$$
$$\{\Gamma, H_{2\mathrm{D}}(k_x,k_y)\} = 0, \quad \Gamma = \tau_z \otimes \sigma_0, \tag{A4}$$

which is topologically nontrivial (trivial) for $-1 < m < 1$ ($m > 1$ or $m < -1$).

The basic idea is as follows: For $H_{1\mathrm{D}}(\boldsymbol{k})$ on $k_x \in S^1$, consider the following two Hamiltonians defined on $(k_x,\theta) \in S^1 \times [0,\pi]$,

$$H_{\mathrm{R}}(k_x,\theta) = \sin\theta\tau_y \otimes H_{1\mathrm{D}}(k_x) + \cos\theta\tau_x \otimes \sigma_0,$$
$$H_{\mathrm{L}}(k_x,\theta) = \sin\theta\tau_y \otimes [-H_{1\mathrm{D}}(k_x)] + \cos\theta\tau_x \otimes \sigma_0, \tag{A5}$$

which are obtained by the isomorphic map (A2). They have the symmetry

$$[U(k_x), H_{\mathrm{R,L}}(k_x,\theta)] = 0, \quad \{\Gamma, H_{\mathrm{R,L}}(k_x,\theta)\} = 0, \tag{A6}$$

with $U(k_x) = \tau_x \otimes \Gamma_{1\mathrm{D}}(k_x)$ and $\Gamma = \tau_z \otimes \sigma_0$. Since $H_{1\mathrm{D}}(k_x)$ and $-H_{1\mathrm{D}}(k_x)$ have different $\boldsymbol{Z}_2$ numbers, either $H_{\mathrm{R}}(k_x,\theta)$ or $H_{\mathrm{L}}(k_x,\theta)$, but not both, is topologically nontrivial. These two Hamiltonians coincide at $\theta = 0$ and π, respectively. Thus, by sewing these two Hamiltonians at $\theta = 0$ and π, as illustrated in Fig. 4, we can obtain a system defined on a two-dimensional torus T^2. The resultant system has a nontrivial $\boldsymbol{Z}_2$ number, which is obtained as the total $\boldsymbol{Z}_2$ numbers of $H_{\mathrm{R}}(k_x,\theta)$ and $H_{\mathrm{L}}(k_x,\theta)$.

To obtain an explicit Hamiltonian of the system on T^2, we change the variable θ as $\theta = \pi/2 - k_y$ in $H_{\mathrm{R}}(k_x,\theta)$ and $\theta = k_y - \pi/2$ in $H_{\mathrm{L}}(k_x,\theta)$, respectively. For the new variable, H_{R} and H_{L} have the same form as $H_{2\mathrm{D}}(k_x,k_y)$,

$$H_{2\mathrm{D}}(k_x,k_y) = \cos k_y \tau_y \otimes H_{1\mathrm{D}}(k_x) + \sin k_y \tau_x \otimes \tau_0, \tag{A7}$$

where H_{L} and H_{R} are smoothly connected at $k_y = \pi/2$ and $k_y = -\pi/2$, respectively. Equation (A7) is the Hamiltonian of the sewn system. Note that we may adiabatically add a term preserving the symmetries (A6) to the Hamiltonian without changing its topological property unless the bulk gap of the system closes. Thus we can finally modify (A7) in the form of Eq. (A3) with $-1 < m < 1$.

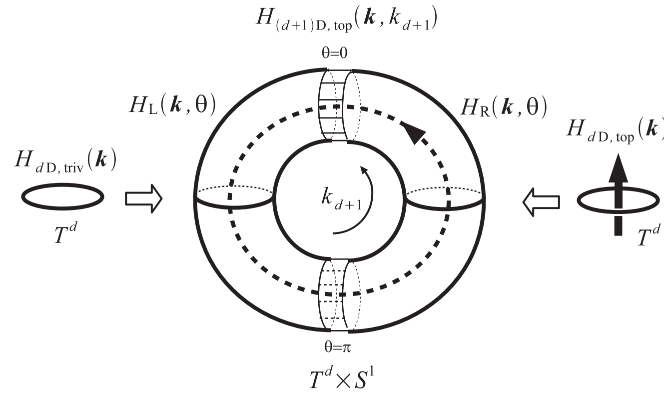

FIG. 4. Hamiltonian mapping. Two Hamiltonians $H_{\mathrm{R}}(\boldsymbol{k},\theta)$ and $H_{\mathrm{R}}(\boldsymbol{k},\theta)$ defined on $T^d \times [0,\pi]$ are sewn at $\theta = 0$ and π.

In a similar manner, we can obtain a system on T^2 with trivial $\boldsymbol{Z}_2$ topology. In this case, we use the same Hamiltonian for $H_{\mathrm{R}}(k_x,\theta)$ and $H_{\mathrm{L}}(k_x,\theta)$,

$$H_{\mathrm{R}}(k_x,\theta) = H_{\mathrm{L}}(k_x,\theta) = \sin\theta\tau_y \otimes H_{1\mathrm{D}}(k_x) + \cos\theta\tau_x \otimes \sigma_0, \tag{A8}$$

with $\theta \in [0,\pi]$. Even when H_{R} and H_{L} have nontrivial $\boldsymbol{Z}_2$ numbers, they are canceled by sewing them at $\theta = 0$ and $\theta = \pi$. An explicit form of the sewn Hamiltonian is obtained as follows. Because $\sin\theta \geqslant 0$, we can add a positive constant m to $\sin\theta$ in Eq. (A8) without gap closing,

$$H_{\mathrm{R}}(k_x,\theta) = H_{\mathrm{L}}(k_x,\theta) = (m + \sin\theta)\tau_y \otimes H_{1\mathrm{D}}(k_x) + \cos\theta\tau_x \otimes \sigma_0, \tag{A9}$$

where we gradually increase m as it satisfies $m > 1$. Then we can adiabatically change the coefficient of $\sin\theta$ in $H_{\mathrm{L}}(k_x,\theta)$ as $\sin\theta \to -\sin\theta$, without gap closing. As a result, H_{R} and H_{L} can be

$$H_{\mathrm{R}}(k_x,\theta) = (m + \sin\theta)\tau_y \otimes H_{1\mathrm{D}}(k_x) + \cos\theta\tau_x \otimes \sigma_0,$$
$$H_{\mathrm{L}}(k_x,\theta) = (m - \sin\theta)\tau_y \otimes H_{1\mathrm{D}}(k_x) + \cos\theta\tau_x \otimes \sigma_0, \tag{A10}$$

with $m > 1$. Finally, by changing the variable θ as $\theta = \pi/2 - k_y$ in $H_{\mathrm{R}}(k_x,\theta)$ and $\theta = k_y - \pi/2$ in $H_{\mathrm{L}}(k_x,\theta)$, respectively, we find that H_{R} and H_{L} have the form of Eq. (A3) with $m > 1$, where H_{R} and H_{L} are smoothly sewn up at $k_y = \pm\pi/2$. We note that if we take the starting Hamiltonians as

$$H_{\mathrm{R}}(k_x,\theta) = H_{\mathrm{L}}(k_x,\theta) = \sin\theta\tau_y \otimes [-H_{1\mathrm{D}}(k_x)] + \cos\theta\tau_x \otimes \sigma_0, \tag{A11}$$

we can obtain Eq. (A3) with $m < -1$, in a similar manner.

The same idea is available to obtain the 3D insulators

$$H_{3\mathrm{D}}(\boldsymbol{k}) = (m + \cos k_z + \cos k_y)\tau_y \otimes H_{1\mathrm{D}}(k_x) + \sin k_y \tau_x \otimes \tau_0 + \sin k_z \tau_z \otimes \tau_0, \tag{A12}$$

with the glide reflection symmetry,

$$G(k_x) H_{3\mathrm{D}}(k_x,k_y,k_z) G^{-1}(k_x) = H_{3\mathrm{D}}(k_x,k_y,-k_z),$$
$$G(k_x) = \tau_x \otimes \Gamma_{1\mathrm{D}}(k_x), \tag{A13}$$

which is $\boldsymbol{Z}_2$ nontrivial ($\boldsymbol{Z}_2$ trivial) for $-2 < m < 0$ or $0 < m < 2$ ($m < -2$ or $m > 2$): Since $H_{\rm 2D}$ in Eq. (A3) is chiral symmetric, we use the isomorphic map (A1) to have $H_{\rm R}(k_x,k_y,\theta)$ and $H_{\rm L}(k_x,k_y,\theta)$,

$$\begin{aligned} H_{\rm R}(k_x,k_y,\theta) &= \sin\theta H_{\rm 2D}(k_x,k_y) + \cos\theta\Gamma, \\ H_{\rm L}(k_x,k_y,\theta) &= \sin\theta H'_{\rm 2D}(k_x,k_y) + \cos\theta\Gamma, \end{aligned} \tag{A14}$$

where we denote $H_{\rm 2D}$ in $H_{\rm L}$ as $H'_{\rm 2D}$ as it can be different from $H_{\rm 2D}$ in $H_{\rm R}$. $H_{\rm R}$ and $H_{\rm L}$ have the same $\boldsymbol{Z}_2$ topological number as $H_{\rm 2D}$ and $H'_{\rm 2D}$, respectively. By jointing $H_{\rm R}$ and $H_{\rm L}$ at $\theta = 0$ and π, we can have a Hamiltonian $H_{\rm 3D}$ defined on a 3D torus T^3. If either $H_{\rm R}$ or $H_{\rm L}$, but not both, is $\boldsymbol{Z}_2$ nontrivial, $H_{\rm 3D}$ is $\boldsymbol{Z}_2$ nontrivial. In other cases, $H_{\rm 3D}$ is $\boldsymbol{Z}_2$ trivial. Then, one can show that with a suitable adiabatic deformation, $H_{\rm 3D}$ takes the form of Eq. (A12) without gap closing.

2. Z_2 invariants for nonsymmorphic systems

1D case

Here we generalize the $\boldsymbol{Z}_2$ invariant defined for the simplest 2×2 Hamiltonian (4) in the main text, to that for the general Hamiltonian.

The nonsymmorphic chiral symmetry is given by

$$\{\Gamma_{\rm 1D}(k_x), H_{\rm 1D}(k_x)\} = 0, \quad \Gamma^2_{\rm 1D}(k_x) = e^{-ik_x}. \tag{A15}$$

By imposing 2π periodicity in k_x on $\Gamma_{\rm 1D}(k_x)$, a general form of $\Gamma_{\rm 1D}(k_x)$ is given by

$$\Gamma_{\rm 1D}(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix} \otimes \boldsymbol{1}_{N\times N}, \tag{A16}$$

with the $N \times N$ unit matrix $\boldsymbol{1}_{N\times N}$. In this basis, the Hamiltonian $H_{\rm 1D}(k_x)$ with the nonsymmorphic chiral symmetry takes the form

$$H_{\rm 1D}(k_x) = \begin{pmatrix} X(k_x) & -iY(k_x)e^{-ik_x/2} \\ iY(k_x)e^{ik_x/2} & -X(k_x) \end{pmatrix}, \tag{A17}$$

where $X(k_x)$ and $Y(k_x)$ are $N \times N$ Hermitian matrices. Since $H_{\rm 1D}(k_x)$ is 2π periodic in k_x, $X(k_x)$ and $Y(k_x)$ satisfy

$$X(k_x + 2\pi) = X(k_x), \quad Y(k_x + 2\pi) = -Y(k_x). \tag{A18}$$

Now we introduce the following $N \times N$ matrix $Z(k_x)$,

$$Z(k_x) = X(k_x) + iY(k_x), \tag{A19}$$

which has the constraint

$$Z(k_x + 2\pi) = Z^\dagger(k_x). \tag{A20}$$

Because one can prove the relation

$$\det H_{\rm 1D}(k_x) = |\det Z(k_x)|^2, \tag{A21}$$

$\det Z(k_x) \neq 0$ when $H_{\rm 1D}(k_x)$ is gapped at $E = 0$ [namely, when $\det H_{\rm 1D}(k_x) \neq 0$].

Denoting the real and imaginary parts of $\det Z(k_x)$ as $x(k_x)$ and $y(k_x)$, respectively, the relation (A21) implies $x^2(k_x) + y^2(k_x) \neq 0$ for a gapped $H_{\rm 1D}(k_x)$. Furthermore, from Eq. (A20), we have

$$x(k_x + 2\pi) = x(k_x), \quad y(k_x + 2\pi) = -y(k_x). \tag{A22}$$

Since $x(k_x)$ and $y(k_x)$ defined here have the same property as those in the main text, we can define the $\boldsymbol{Z}_2$ invariant in the same manner.

As shown in the main text, the simplest Hamiltonian with the nontrivial $\boldsymbol{Z}_2$ invariant is $H_{\rm o} = -\sigma_z$, which gives $[x(k_x), y(k_x)] = (-1,0)$. To confirm the $\boldsymbol{Z}_2$ nature, consider the direct sum $H_{\rm o} \oplus H_{\rm o}$. In the basis where $\Gamma_{\rm 1D}(k_x)$ takes the form of Eq. (A16), $H_{\rm o} \oplus H_{\rm o}$ gives $X(k_x) = -\boldsymbol{1}_{2\times 2}$ and $Y(k_x) = 0$. Thus, we find $[x(k_x), y(k_x)] = (1,0)$ for $H_{\rm o} \oplus H_{\rm o}$, which implies that $H_{\rm o} \oplus H_{\rm o}$ is $\boldsymbol{Z}_2$ trivial.

3. 2D case

In this section, we define the $\boldsymbol{Z}_2$ invariant for the 2D Hamiltonian which has the nonsymmorphic symmetry

$$[U(k_x), H_{\rm 2D}(k_x,k_y)] = 0, \quad U(k_x)^2 = e^{-ik_x}, \tag{A23}$$

as well as the ordinary chiral symmetry,

$$\{H_{\rm 2D}(k_x,k_y), \Gamma\} = 0, \quad \Gamma^2 = 1. \tag{A24}$$

These symmetries anticommute,

$$\{\Gamma, U(k_x)\} = 0. \tag{A25}$$

Consider the Schrödinger equation given by

$$H_{\rm 2D}(k_x,k_y)|u_n(k_x,k_y)\rangle = E_n(k_x,k_y)|u_n(k_x,k_y)\rangle, \tag{A26}$$

where n is the band index. We assume that the system is gapped at $E = 0$, and the Fermi energy is inside the gap. It is convenient here to use a positive (negative) n to represent a positive (negative) energy band.

Since $H_{\rm 2D}(k_x,k_y)$ commutes with $U(k_x)$, the solutions $|u_n(k_x,k_y)\rangle$ are taken as eigenstates of $U(k_x)$

$$U(k_x)|u_n^\pm(k_x,k_y)\rangle = \pm e^{-ik_x/2}|u_n^\pm(k_x,k_y)\rangle. \tag{A27}$$

The chiral symmetry implies that if $|u_n^\pm(k_x,k_y)\rangle$ is a positive (negative) energy band, $\Gamma|u_n^\pm(k_x,k_y)\rangle$ is a negative (positive) energy band. From the anticommutation relation (A25), it is also found that $\Gamma|u_n^\pm(k_x,k_y)\rangle$ is an eigenstate of $U(k_x)$ with the eigenvalue $\mp e^{ik_x/2}$. Therefore, we can place the relation

$$|u_n^\pm(k_x,k_y)\rangle = \Gamma|u_{-n}^\mp(k_x,k_y)\rangle. \tag{A28}$$

A key character of the nonsymmorphic symmetry $U(k_x)$ is that its eigenvalues $\pm e^{-ik_x/2}$ do not have the same periodicity as $U(k_x)$ itself: They change their sign when $k_x \to k_x + 2\pi$. As a result, $|u_n^+(k_x,k_y)\rangle$ and $|u_n^-(k_x + 2\pi,k_y)\rangle$ have the same eigenvalue of $U(k_x)$, satisfying the same Schrödinger equation. Thus, they are the same state up to a $U(1)$ gauge factor,

$$|u_n^+(k_x + 2\pi,k_y)\rangle = e^{i\theta_n(k_x,k_y)}|u_n^-(k_x,k_y)\rangle. \tag{A29}$$

This relation gives a nontrivial relation in Berry phases: Introducing the gauge field in the momentum space,

$$A_i^\pm(k_x,k_y) = i\sum_{n<0}\langle u_n^\pm(k_x,k_y)|\partial_{k_i}u_n^\pm(k_x,k_y)\rangle, \tag{A30}$$

we define the Berry phases $\gamma^{\pm}(k_x)$ as

$$e^{i\gamma^{\pm}(k_x)} = \exp\left(i \oint dk_y A_y^{\pm}(k_x,k_y)\right). \quad \text{(A31)}$$

Since Eq. (A29) implies

$$A_i^{\pm}(k_x+2\pi,k_y) = A_i^{\mp}(k_x,k_y) - \sum_{n<0} \partial_{k_i}\theta_n(k_x,k_y), \quad \text{(A32)}$$

the Berry phases satisfy

$$e^{i\gamma^{+}(k_x+2\pi)} = e^{i\gamma^{-}(k_x)} e^{-i\oint dk_y \sum_{n<0} \partial_{k_y}\theta_n(k_x,k_y)}. \quad \text{(A33)}$$

From the periodicity in k_y, the integral $\oint dk_y \partial_{k_y}\theta_n$ should be $2\pi N_n$ with an integer N_n, and thus we have

$$e^{i\gamma^{+}(k_x+2\pi)} = e^{i\gamma^{-}(k_x)}. \quad \text{(A34)}$$

Now we use Eq. (A28). This equation implies

$$A_i^{+}(k_x,k_y) + A_i^{-}(k_x,k_y) = i\sum_n \langle u_n^{+}(k_x,k_y)|\partial_{k_i} u_n^{+}(k_x,k_y)\rangle, \quad \text{(A35)}$$

where the summation in the right-hand side is taken for all n. Therefore, from the completeness relation, we find that $A_i^{+}(k_x,k_y) + A_i^{-}(k_x,k_y)$ is a total derivative of a function, which yields

$$e^{i[\gamma^{+}(k_x)+\gamma^{-}(k_x)]} = 1. \quad \text{(A36)}$$

Combining this with Eq. (A34), we finally have

$$e^{i\gamma^{+}(k_x+2\pi)} = e^{-i\gamma^{+}(k_x)}. \quad \text{(A37)}$$

Using this relation, we can define the $\boldsymbol{Z}_2$ invariant in the same manner as the 1D case: Denoting the real and imaginary parts of $e^{i\gamma^{+}(k_x)}$ as $x(k_x)$ and $y(k_x)$, respectively, we can introduce a nonzero two-dimensional vector $[x(k_x),y(k_x)]$. Then Eq. (A37) gives the constraint

$$x(k_x+2\pi) = x(k_x), \quad y(k_x+2\pi) = -y(k_x), \quad \text{(A38)}$$

which is exactly the same as Eq. (5). Therefore, if the trajectories $[x(k_x),y(k_x)]$ passes the positive x axis an odd (even) number of times, the system is topologically nontrivial (trivial).

The $\boldsymbol{Z}_2$ invariant of the Hamiltonian (7) is evaluated as follows. It is sufficient to consider the case with $H_{1\mathrm{D}}(k_x) = \sigma_z$ since $H_{1\mathrm{D}}(k_x)$ can deform into σ_z without gap closing. $H_{2\mathrm{D}}(k_x,k_y)$ is block diagonal in the diagonal basis of $U(k_x)$, and in the sector with the eigenvalue $u = \pm e^{-ik_x/2}$ of $U(k_x)$, it is given by

$$H_{2\mathrm{D}}^{\pm} = \pm\begin{pmatrix} \sin k_y & i(m+\cos k_y) \\ -i(m+\cos k_y) & -\sin k_y \end{pmatrix}. \quad \text{(A39)}$$

From this, we obtain

$$\gamma^{\pm}(k_x) = \begin{cases} 0 & \text{for} \quad m < -1 \\ \pi & \text{for} \quad -1 < m < 1 \\ 0 & \text{for} \quad m > 1, \end{cases} \quad \text{(A40)}$$

which implies the $\boldsymbol{Z}_2$ invariant is nontrivial (trivial) if $-1 < m < 1$ ($m > 1$ or $m < -1$).

4. 3D case

Finally, we define the $\boldsymbol{Z}_2$ topological invariant associated with glide symmetry

$$G(k_x)H_{3\mathrm{D}}(k_x,k_y,k_z)G^{-1}(k_x) = H_{3\mathrm{D}}(k_x,k_y,-k_z),$$
$$G^2(k_x) = e^{-ik_x}. \quad \text{(A41)}$$

From solutions of the Schrödinger equation

$$H_{3\mathrm{D}}(\boldsymbol{k})|u_n(\boldsymbol{k})\rangle = E_n(\boldsymbol{k})|u_n(\boldsymbol{k})\rangle, \quad \text{(A42)}$$

we introduce the gauge field $A_i(\boldsymbol{k})$ in the momentum space,

$$A_i(\boldsymbol{k}) = i\sum_{E_n(\boldsymbol{k})<E_{\mathrm{F}}} \langle u_n(\boldsymbol{k})|\partial_{k_i} u_n(\boldsymbol{k})\rangle, \quad \text{(A43)}$$

where E_{F} is the Fermi energy. On the glide invariant plane at $k_z = \Lambda$ ($\Lambda = 0,\pi$), the glide operator $G(k_x)$ commutes with $H_{3\mathrm{D}}$,

$$[G(k_x), H_{3\mathrm{D}}(k_x,k_y,\Lambda)] = 0, \quad \text{(A44)}$$

and thus the solutions of the Schrödinger equation are simultaneously eigenstates of $G(k_x)$,

$$G(k_x)|u_n^{\pm}(k_x,k_y,\Lambda)\rangle = \pm e^{-ik_x/2}|u_n^{\pm}(k_x,k_y,\Lambda)\rangle. \quad \text{(A45)}$$

Correspondingly, we can decompose $A_i(\boldsymbol{k})$ into two parts,

$$A_i(k_x,k_y,\Gamma) = A_i^{+}(k_x,k_y,\Lambda) + A_i^{-}(k_x,k_y,\Lambda) \quad \text{(A46)}$$

with

$$A_i^{\pm}(k_x,k_y,\Lambda) = i\sum_{E_n<E_{\mathrm{F}}} \langle u_n^{\pm}(k_x,k_y,\Lambda)|\partial_{k_i} u_n^{\pm}(k_x,k_y,\Lambda)\rangle. \quad \text{(A47)}$$

In a manner similar to $U(k_x)$ in 2D, the eigenvalues of $G(k_x)$ do not have the same periodicity in k_x as $G(k_x)$ itself, and they change their sign when $k_x \to k_x + 2\pi$. As a result, we have a twisted boundary condition,

$$|u_n^{\pm}(k_x+2\pi,k_y,\Lambda)\rangle = e^{i\theta_n^{\pm}(k_x,k_y,\Lambda)}|u_n^{\mp}(k_x,k_y,\Lambda)\rangle, \quad \text{(A48)}$$

where $\theta_n^{\pm}(k_x,k_y,\Lambda)$ is a $U(1)$ phase.

Now we consider the upper half region of the Brillouin zone in Fig. 5. From the twisted boundary condition, the Berry phases $\gamma^{\pm}(\ell)$ along $\ell = a,b,c,d$ in Fig. 5,

$$\gamma^{\pm}(\ell) = \oint_{\ell} dk_y A_y^{\pm}(k_x,k_y,\Lambda) \quad \text{(A49)}$$

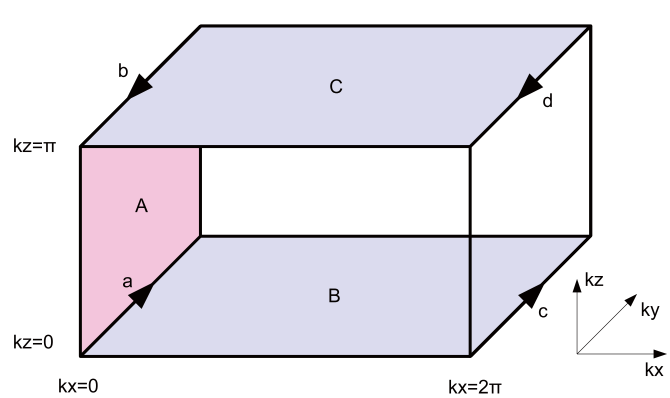

FIG. 5. (Color online) Upper half Brillouin zone.

satisfy

$$\begin{aligned}\gamma^+(a) &= \gamma^-(c) \pmod{2\pi},\\ \gamma^+(b) &= \gamma^-(d) \pmod{2\pi}.\end{aligned} \tag{A50}$$

The Stokes' theorem also leads to

$$\begin{aligned}\gamma(a+b) &= \int_A F_{yz} dk_y dk_z \pmod{2\pi},\\ \gamma^\pm(c-a) &= \int_B F^\pm_{xy} dk_x dk_y \pmod{2\pi},\\ \gamma^\pm(b-d) &= \int_C F^\pm_{xy} dk_x dk_y \pmod{2\pi},\end{aligned} \tag{A51}$$

with $\gamma(\ell) = \gamma^+(\ell) + \gamma^-(\ell)$, $F_{yz} = \partial_{k_y} A_z - \partial_{k_y} A_z$, and $F^\pm_{xy} = \partial_{k_x} A^\pm_y - \partial_{k_y} A^\pm_x$. The modular equality in the above equations comes from the ambiguity of the Berry phases.

Using these relations, we find that the following ν defines the $\mathbf{Z}_2$ invariant $(-1)^\nu$:

$$\begin{aligned}\nu = \frac{1}{2\pi}\left[\int_A F_{yz} dk_y dk_z + \int_{B-C} F^-_{xy} dk_x dk_y\right]\\ - \frac{1}{\pi}\gamma^+(a+b) \pmod 2.\end{aligned} \tag{A52}$$

Here note that the modulo-2 ambiguity from the Berry phase $\gamma^+(a+b)$ does not affect the $\mathbf{Z}_2$ invariant $(-1)^\nu$. In order for $(-1)^\nu$ to define the $\mathbf{Z}_2$ invariant, ν must be an integer. From Eqs. (A51) and (A50), we find that

$$\begin{aligned}&\frac{1}{2\pi}\int_{B-C} F^-_{xy} dk_x dk_y\\ &= \frac{1}{2\pi}\gamma^-(c-a-b+d)\\ &= \frac{1}{2\pi}[\gamma^-(c+d) - \gamma^-(a+b)]\\ &= \frac{1}{2\pi}[\gamma^+(a+b) - \gamma^-(a+b)] \pmod 1.\end{aligned} \tag{A53}$$

Therefore, ν is recast into

$$\nu = \frac{1}{2\pi}\left[\int_A F_{yz} dk_y dk_z - \gamma(a+b)\right] \pmod 1, \tag{A54}$$

which takes an integer.

From the formula (A52), we can calculate the $\mathbf{Z}_2$ invariant $(-1)^\nu$ for $H_{3\mathrm{D}}(\boldsymbol{k})$ in Eq. (14). Since the $\mathbf{Z}_2$ invariant takes the same value unless the gap of the system closes, we can choose the special case of $H_{1\mathrm{D}}(k_x) = \sigma_z$. In this case, the first and the second terms of the right-hand side of Eq. (A52) vanish, and thus we only need to evaluate $\gamma^+(a+b)$. On the glide invariant plane at $k_z = \Lambda$, $H_{3\mathrm{D}}(k_x,k_y,\Lambda)$ is decomposed into $H^\pm_{3\mathrm{D}}$ in the sector with the eigenvalue $\pm e^{-ik_x/2}$ of $G(k_x)$,

$$\begin{aligned}&H^\pm_{3\mathrm{D}}(k_x,k_y,\Lambda)\\ &= \pm\begin{pmatrix}\sin k_y & i(m+\cos\Lambda+\cos k_y)\\ -i(m+\cos\Lambda+\cos k_y) & -\sin k_y\end{pmatrix}.\end{aligned} \tag{A55}$$

From this, we find that

$$\begin{aligned}\gamma^+(a) &= \begin{cases}0 & \text{for } m<-2\\ \pi & \text{for } -2<m<0\\ 0 & \text{for } m>0,\end{cases}\\ \gamma^+(b) &= \begin{cases}0 & \text{for } m<0\\ \pi & \text{for } 0<m<2\\ 0 & \text{for } m>2,\end{cases}\end{aligned} \tag{A56}$$

which implies

$$\nu = \begin{cases}0 & \text{for } m<-2\\ 1 & \text{for } -2<m<0\\ 1 & \text{for } 0<m<2\\ 0 & \text{for } m>2,\end{cases} \tag{A57}$$

modulo 2. Therefore, $H_{3\mathrm{D}}(\boldsymbol{k})$ in Eq. (14) is topologically nontrivial (trivial) if $-2<m<0$ or $0<m<2$ ($m>1$ or $m<-1$).

5. K-theory analysis

We summarize relevant results in the K theory. Consider a class of nonsymmorphic symmetries, $\{U|\tau_x\}$, which consist of a point group operation U accompanying a half translation τ_x of the lattice spacing in the x direction. We assume that the point group operation U is a $\mathbb{Z}_2$ transformation (namely, order two). The nonsymmorphic symmetry $\{U|\tau_x\}$ acts on the Bloch Hamiltonian $H(\boldsymbol{k})$ as a k_x-dependent unitary transformation $U(k_x)$ with $U^2(k_x) = e^{-ik_x/2}$.

Let us denote the K group for d-dimensional insulators with the nonsymmorphic symmetry $U(k_x)$ as $K^{(s,t,\tau_x)}_{\mathbb{Z}_2}(T^d)$. Here the superscript (s,t,τ_x) identifies the symmetries of the insulators: $s = 0,1 \pmod 2$ indicates the absence ($s=0$) or the presence ($s=1$) of the additional chiral symmetry. Then $t = 0,1 \pmod 2$ determines how the point group operation of $U(k_x)$ acts; for $s=0$, t specifies the action of $U(k_x)$ as [36]

$$U(k_x)H(k_x,\boldsymbol{k})U(k_x)^{-1} = \begin{cases}H(k_x,\tilde{\boldsymbol{k}}) & (t=0)\\ -H(k_x,\tilde{\boldsymbol{k}}) & (t=1),\end{cases} \tag{A58}$$

and for $s=1$,

$$\begin{aligned}&\{H(k_x,\boldsymbol{k}),\Gamma\} = 0, \quad U(k_x)H(k_x,\boldsymbol{k})U(k_x)^{-1} = H(k_x,\tilde{\boldsymbol{k}}),\\ &\Gamma U(k_x) = \begin{cases}U(k_x)\Gamma & (t=0)\\ -U(k_x)\Gamma & (t=1),\end{cases}\end{aligned} \tag{A59}$$

where $\boldsymbol{k}\mapsto\tilde{\boldsymbol{k}}$ represents a $\mathbb{Z}_2$ transformation for T^{d-1}. Finally, τ_x represents the half translation in the x direction, as mentioned above. (t,τ_x) is an example of a twisting of the twisted equivariant K theory for topological insulators and superconductors [44].

From the Gysin exact sequence [45] in the K theory (the twisted version follows from the Thom isomorphism theorem [46]), for S^1 except in the k_x direction, the following isomorphism can be shown:

$$K^{(s,t,\tau_x)}_{\mathbb{Z}_2}(T^d\times S^1) \cong K^{(s,t,\tau_x)}_{\mathbb{Z}_2}(T^d) \oplus K^{(s-1,t,\tau_x)}_{\mathbb{Z}_2}(T^d), \tag{A60}$$

if $U(k_x)$ for $K^{(s,t,\tau_x)}_{\mathbb{Z}_2}(T^d\times S^1)$ acts on S^1 as a global symmetry, or

$$K^{(s,t,\tau_x)}_{\mathbb{Z}_2}(T^d\times S^1) \cong K^{(s,t,\tau_x)}_{\mathbb{Z}_2}(T^d) \oplus K^{(s-1,t-1,\tau_x)}_{\mathbb{Z}_2}(T^d), \tag{A61}$$

if $U(k_x)$ for $K_{\mathbb{Z}_2}^{(s,t,\tau_x)}(T^d \times S^1)$ acts on S^1 as a reflection symmetry. By iterating Eqs. (A60) and (A61), any K group in the present case reduces to that for a one-dimensional nonsymmorphic insulator defined in the k_x direction. The Hamiltonian mapping $d = 1 \to d = 2 \to d = 3$ discussed previously is based on the isomorphism (A60) and (A61). In Eq. (A60) or (A61), the first term $K_{\mathbb{Z}_2}^{(n,t,\tau_x)}(T^d)$ in the right-hand side represents a "weak" topological index of the left-hand side, which is obtained by just neglecting the S^1 dependence in the left-hand side, but the second term gives the "strong" topological index.

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