Effective field theories of topological crystalline insulators and topological crystals

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We present a general approach to obtain effective field theories for topological crystalline insulators whose low-energy theories are described by massive Dirac fermions. We show that these phases are characterized by the responses to spatially dependent mass parameters with interfaces. These mass interfaces implement the dimensional reduction procedure such that the state of interest is smoothly deformed into a *topological crystal*, which serves as a representative state of a phase in the general classification. Effective field theories are obtained by integrating out the massive Dirac fermions, and various quantized topological terms are uncovered. Our approach can be generalized to other crystalline symmetry-protected topological phases and provides a general strategy to derive effective field theories for such crystalline topological phases.

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I. INTRODUCTION

Topological phases of matter are gapped phases which are characterized by the patterns of quantum entanglement in the ground state [1]. A ground state with a short-range quantum entanglement is considered trivial since the state can be smoothly deformed into a product state of microscopic degrees of freedom without closing the energy gap. Such deformation might not be possible in the presence of symmetry, allowing us to define the so-called symmetry-protected topological (SPT) phases [2–15]. Explicitly, a SPT phase is a gapped phase of matter with a unique ground state that cannot be adiabatically deformed to a trivial state as long as the symmetry is preserved; the adiabatic trivialization is possible only if the symmetry is allowed to be broken.

For internal symmetries, general understanding of SPT phases has been largely achieved [16–19]. Aside from the development of SPT phases with internal symmetries, there has been a great interest on topological phases with crystalline point-group and space-group symmetries [20–26]. Typical examples include so-called topological crystalline insulators (TCIs), which are electronic insulators protected, in part, by point-group or space-group symmetries [27–29]. As a consequence of crystalline symmetry, higher-order topology may occur in crystalline SPT (cSPT) phases, where anomalous gapless modes could show up on the $(d-n)$-dimensional boundary of a d-dimensional bulk (with $n>1$) [30,31].

There have been two general frameworks which are conjectured to give a general classification of cSPT phases. The first are dubbed the "topological crystal" approach [32–46], in which the key idea is to deform a generic cSPT state into a real-space stacking of "building blocks," which are lower-dimensional SPT states with effective internal symmetry. These special kinds of states are referred to as topological crystals. The classification of cSPT phases is then given by the deformation classes of the topological crystals. This approach gives a simple physical picture for understanding cSPT phases. Interesting physical signatures on the boundaries [47,48] or crystalline defects [46] are usually easy to obtain in this framework.

The second framework is based on the "smooth states" [49]. In this framework, a hypothetical lattice of ancillas (hypothetical degrees of freedom) is introduced, and the lattice of ancillas has a much smaller lattice constant than the physical lattice. A smooth state is very smooth in the lattice of ancillas. However, the radius of the spatial variation of a smooth state is on the order of the unit-cell size of the physical lattice. An important consequence in this framework is that the classification of cSPT phases with a crystalline symmetry group G is the same as the classification of SPT phases with internal symmetry group G, which is known as the "crystalline equivalence principle" (see also Refs. [50–52]). The topological crystal and the smooth state approach are actually equivalent as shown in Ref. [53].

In principle, SPT phases should be characterized by their response to background gauge fields. The concept of crystalline gauge fields has been mathematically defined [49], but the result is rather formal, which limits the practical usage. Further attempts have been made in order to turn it into a concrete theoretical tool either in the field-theory framework [54–56] or on the lattice [56]. There has been an alternative proposal which characterizes cSPT phases through their response to elastic deformations [57–61]. This approach is very physical and is well defined in a continuous field theory. However, it has only been worked out in some simple examples, and the relation to the general classification can only be obtained formally. It is also unclear how to derive such effective field theories microscopically.

In this paper, we propose a continuous field-theoretical description of the cSPT phases. Focusing on TCIs described by

massive Dirac theories, the main idea is to characterize these phases by the responses to spatially dependent mass parameters (and to the background gauge field of internal symmetry). These spatially dependent mass terms implement the dimensional reduction procedure such that the states trapped at the mass interfaces are precisely the building blocks in the corresponding topological crystal picture. The effective field theory is then obtained by integrating out the gapped fermions. Our approach not only provides well-defined effective field theories for the cSPT phases, but also gives an explicit connection between the topological crystal picture and the effective field theories.

The rest of this paper is organized as follows: In Sec. II, we give a review of the topological crystal approach and summarize our main results. Cellular cohomology is used throughout this paper, which we review in Appendix A.

In Sec. III, we discuss the effective field theory for one-dimensional (1D) atomic insulators with charge conservation and the lattice translation symmetry as a simple example to illustrate our approach. Generalizations to two- and three-dimensional (2D and 3D) atomic insulators are also discussed and more details are given in Appendix D. We point out that the responses described by these topological terms are generalized Thouless pumps.

In Sec. IV, we apply our approach to various TCIs with point-group symmetry and derive the effective field theories. Section IV A considers 1D TCIs with reflection symmetry. Section IV B generalizes the discussion to 2D TCIs with C_N rotational symmetry. Since the form of the topological term for this case might not be familiar to the readers, we provide a perturbative derivation in Appendix E. Section IV C is devoted to 3D second-order TCIs protected by C_{nv} symmetry, where there are gapless hinge modes for appropriate boundary conditions. The field theories we obtained are essentially the same as the axion field theory [62], where the nontrivial information of the classification is encoded in the theta angle. We also briefly discuss the physical responses as the a result of the topological terms in the effective field theories.

Finally, we conclude in Sec. V with a discussion of our results and possible directions for future work. Other mathematical details are given in Appendix B, including general discussions on the fundamental domain for crystalline symmetry, and the construction of the map $f : M \to BG_s$, where M is the real-space manifold and the BG_s is the classifying space for the space group G_s. Appendix C gives a construction of the classifying space BG_s for a space group.

II. GENERAL PERSPECTIVE AND SUMMARY OF THE RESULTS

A. Review of the topological crystal approach

Topological crystal approach is a general framework of describing and classifying cSPT phases. The main idea is that any cSPT phase is adiabatically connected to a stacking of d_b-dimensional topological states with effective internal symmetry arranged in some crystalline pattern in d-dimensional space, where d_b ranges from 0 to d. This procedure is called dimensional reduction and these special kinds of states are referred to as the topological crystals in Ref. [39]. In order for the argument to go through, an important assumption is that the correlation length ξ can be tuned to be arbitrarily small, and, in the presence of translation symmetry, much smaller than the size of the unit cell, which requires adding a fine mesh of trivial degrees of freedom.

A systematic way to describe a topological crystal is as follows. We define a fundamental domain (FD) to be a smallest simply connected closed part of space, subject to the condition that no two points in the region are related by a crystalline symmetry. The FD is then copied throughout space using the crystalline symmetry such that the whole of space is filled. A more formal definition of the FD is given in Appendix B. This construction gives a d-dimensional space a cell complex structure, where the d cells are copies of FD. The $(d-1)$ cells lie on faces where two d cells meet, with the property that no two points in the same $(d-1)$ cell are related by symmetry. This procedure continues to 0 cells. As shown in Appendix B, an important property of this cell complex is that there exists a map $f : M \to BG_s$, where BG_s is the classifying space of the space group G_s. A construction of the classifying space BG_s is given in Appendix C. As a result, each d cell can be labeled by a group element in the space group, and each path connecting a point $\boldsymbol{r}$ in a FD to $g\boldsymbol{r}$ is also labeled by a group element $g \in G_s$.

With this cell-complex structure, one can understand a topological crystal state by associating d_b-dimensional topological phase with each d_b cell. These d_b-dimensional states are referred to as the "building blocks" of the topological crystal. When the building blocks intersect in the bulk, the building blocks must be glued together so as to eliminate any gapless modes at the junctions while preserving symmetry. An ordinary crystal is a simple example of a topological crystal state, which is formed by periodically arranged atoms as $d_b = 0$ building blocks.

B. Characterizing topological crystalline phases by responses to mass parameters

In this section, we summarize general aspects of our approach on deriving the effective field theories for cSPT phases. The main idea of this work is to characterize cSPT phases by their response to spatially dependent mass parameters. These spatially dependent mass terms have interfaces that implement the dimensional reduction procedure such that the states trapped at the mass interfaces are precisely the building blocks in the corresponding topological crystal picture. The effective field theory is then obtained by integrating out the gapped fermions. This provides a way to connect the topological crystal picture to the effective field theories.

One of the simplest examples is given in a one-dimensional crystal with a lattice translation symmetry and a U(1) charge conservation symmetry. There is an integer topological invariant ν representing the charge per unit cell. We will show that the topological response of such a system to a spatially dependent mass parameter background and to a background U(1) gauge field A_μ is characterized by a quantized topological term

$$\frac{\nu}{2\pi}\int \epsilon^{\mu\nu}A_\mu\partial_\nu\phi(x)d^2x, \tag{1}$$

where $\phi(x)$ is a phase variable that parametrizes the winding of the mass interface. The charge-ν bound state trapped at the mass interface with a nontrivial $2\pi\nu$ winding is precisely the $d_b = 0$ building block in the topological crystal picture of this phase. Detailed arguments and the derivation are given in Sec. III.

In order for this approach to make sense, it is important to consider the "topological limit," where one tunes the correlation length ξ to be arbitrarily small, especially $\xi \ll a$ (where a is the size of a unit cell) in the presence of lattice translation symmetry. One can imagine that the system is defined on a much finer lattice with lattice spacing $l \ll a$. It is still possible to describe a system in the topological limit by a continuous field theory. One considers fields that are coarse grained with respect to the length scale l so that the fields are smooth on the scale l and could vary on the scale R with $R \gg l$ and $R < a$. Working in the topological limit, the translation symmetry can not be viewed as an effective internal symmetry of the field theory. This property emerges only when one goes to the true "IR limit," where the fields are smooth even on the scale a. In the topological limit, it thus makes sense to consider a mass interface with a characteristic length scale $w < a$ so that the dimensional reduction procedure goes through. In this paper, we will first derive the topological terms in the topological limit. Once a topological term is obtained, we are free to deform the field configurations of the mass parameters to be smooth on the scale a while staying in the same classification class. The resulting theory will be validated in the IR limit. This is the general perspective that we take in this work.

C. Summary of the results

Ideally we would like to apply this method to obtain the quantized topological terms for any cSPT phase. However, doing this in full generality is still a difficult task. In this work, we instead illustrate our approach in physically relavant systems. We consider a wide range of TCIs in one, two, and three dimensions with a U(1) charge conservation and a G_c crystalline symmetry. For simplicity, we consider TCIs that can be built from building blocks with only charge U(1) response, i.e., the building blocks are d_b-dimensional topological phases with U(1) symmetry, which transform trivially under G_c. These building blocks are characterized by the Chern-Simons term

$$\mathcal{L}_{\rm CS}^{2s+1}[A] = \frac{1}{(s+1)!} A \wedge \left(\frac{dA}{2\pi}\right)^s, \tag{2}$$

where A is the U(1) gauge field. For these examples, we find the quantized topological terms take the following general form:

$$S = \int \mathcal{L}_{\rm CS}^{d-k+1}[A] \wedge \Omega_k, \tag{3}$$

where d is spatial dimension and Ω_k is a k form that corresponds to the codimension-k mass interfaces at which the building blocks are decorated. We will show that the mass interfaces that implement the dimensional reduction procedure are classified by $H^k(BG_c, \mathbb{Z})$ with a twisting coefficient when G_c contains orientation reversing elements. The k form Ω_k in the topological term (3) is given by $\Omega_k = f^*\alpha$, where f is the map $f : M \to BG_c$ given by the FDs in crystallography and $\alpha \in H^k(BG_c, \mathbb{Z})$. In general, the k form Ω_k is determined by a set of integral relations, which take the following form:

$$\int_{C_{\{g\}}} \Omega_k = N_{\{g\}}, \tag{4}$$

where $C_{\{g\}}$ is a k cycle labeled by a set of group elements $\{g\}$ in G_c, and $N_{\{g\}}$ is given by

$$N_{\{g\}} = \int_{C_{\{g\}}} f^*\alpha \tag{5}$$

with $\alpha \in H^k(BG_c, \mathbb{Z})$. Here $N_{\{g\}}$ is in general an integer or a $\mathbb{Z}_n$ number depending the cohomology group $H^k(BG_c, \mathbb{Z})$. We note that, in all the examples considered in this work, it is enough to use a single group element $g \in G_c$ to label the k cycle. Representative of Ω_k can be obtained by solving these equations. Table I summarizes the examples and the results in this work. From the topological term (3), one can obtain electromagnetic responses of TCIs, which will be briefly discussed in the sections of each case.

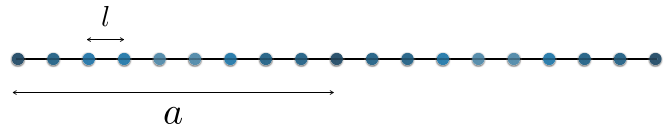

FIG. 1. A 1D lattice of ancillas with lattice spacing l much smaller than the unit-cell size a. The correlation length ξ is assumed to be much less than the unit cell a. After coarse graining with respect to the lattice space l, local observables have spatial variation within the unit cell. The original atoms are represented as the charge density wave (gradient blue colors) in the lattice of ancillas.

III. WARMUP: EFFECTIVE FIELD THEORIES OF 1D ATOMIC INSULATORS

To illustrate the basic idea, we begin with a simple example: 1D atomic insulators. The relevant symmetry group is $\mathrm{U}(1) \times \Gamma$, where U(1) is the charge conservation symmetry and $\Gamma \cong \mathbb{Z}$ is a 1D discrete translation symmetry. Fermion parity is the $\mathbb{Z}_2$ subgroup of U(1). We will focus on such a 1D atomic insulator whose building block picture has a charge-1 atom per unit cell.

A model of a 1D atomic insulator consisting of spinless fermions on a 1D lattice with unit-cell size a so that there is a unit charge per unit cell. We then consider a much finer lattice by adding degrees of freedom as ancillas within each unit cell. Note that these ancillas are not the physical atoms. This setup is shown in Fig. 1. The new model, which has a lattice spacing $l \ll a$,[1] is described by the Hamiltonian

$$H = -t \sum_x^L (c_x c_{x+l}^\dagger + \text{H.c.}) - \mu \sum_x^L c_x^\dagger c_x + \cdots, \tag{6}$$

[1]To simplify the analysis, here we choose $a/l = 2m$ with $m \gg 1$ without loss of generality. One is free to choose a/l to be an odd integer, which will not affect the results.

TABLE I. Summary of the results. The second column specified the symmetry group of the system. Γ, D_1, C_N, C_{nv} denote lattice translation, reflection, N-fold rotation, and C_{nv} point group, respectively. The third column gives the k form Ω_k that appears in the topological term (3). The fourth column lists the integral conditions that Ω_k needs to be satisfied. Here we use t_I, g_r, and u to denote the generator of the lattice translation in the Ith direction, reflection, and the N-fold rotations, respectively. A 1-cycle labeled by g is denoted by C_g, and the 2-cycle labeled by the generator of the N-fold rotation u is denoted by D_u, of which the boundary is given by N 1-cycles C_u. The last column shows the section of the paper where each case is discussed.

Space-time dimensions	Symmetry group G	Ω_k in Eq. (3)	Integral conditions	Section
$(1+1)$D	$U(1)\times\Gamma$	$\Omega_1 = E$	$\int_{C_{t_1}} E = \int_{C_{t_1}} f^*\tau \in \mathbb{Z}, \tau \in H^1(B\Gamma,\mathbb{Z})$	Sec. III
$(1+1)$D	$U(1)\times D_1$	$\Omega_1 = dP$	$\int_{C_{g_r}} dP = \int_{C_{g_r}} f^*r \in \mathbb{Z}_2, r \in H^1(BD_1,\mathbb{Z}^r)$	Sec. IV A
$(2+1)$D	$U(1)\times\Gamma$	$\Omega_2 = \frac{1}{2}\epsilon_{IJ}E^I\wedge E^J$	$\int_{C_{t_I}} E^I = \int_{C_{t_I}} f^*\tau^I \in \mathbb{Z}, \tau^I \in H^1(BT_I,\mathbb{Z})$	App. D
$(2+1)$D	$U(1)\times C_N$	$\Omega_2 = d\omega_1$	$\int_{D_u} d\omega_1 = \int_{D_u} f^*b \in \mathbb{Z}_N, b \in H^2(BC_N,\mathbb{Z})$	Sec. IV B
$(3+1)$D	$U(1)\times\Gamma$	$\Omega_3 = \frac{1}{6}\epsilon_{IJK}E^I\wedge E^J\wedge E^K$	$\int_{C_{t_I}} E^I = \int_{C_{t_I}} f^*\tau^I \in \mathbb{Z}, \tau^I \in H^1(BT_I,\mathbb{Z})$	App. D
$(3+1)$D	$U(1)\times C_{nv}$	$\Omega_1 = dP^{(n)}$	$\int_{C_{g_r}} dP^{(n)} = \int_{C_{g_r}} f^*r \in \mathbb{Z}_2, r \in H^1(BD_1,\mathbb{Z}^r)$ $\int_{C_u} dP^{(n)} = \int_{C_u} f^*a = 0, a \in H^1(BC_N,\mathbb{Z})$	Sec. IV C

where x labels the ancillas. The ellipsis represents various perturbations consistent with the U(1) and the translation symmetries Γ while preserving the average charge per unit cell. The translation symmetry acts on the fermions by

$$t : c_x \to c_{x+a}. \tag{7}$$

By construction, the new model also has the charge U(1) and translation symmetry Γ.

Now we want to derive the continuum IR limit of the theory where the fields are coarse grained with respect to the lattice spacing l. To proceed, we expand the microscopic fermion operator c_x in terms of the slowly varying low-energy fields $\psi_{R/L}$ as

$$c_x \sim \psi_R(x)e^{ik_F x} + \psi_L(x)e^{-ik_F x}, \tag{8}$$

where $k_F = \pi/l$. Define $\psi(x) = (\psi_R, \psi_L)^T$ as the low-energy fermion field, the continuum IR limit of the theory takes the following general form:

$$\mathcal{L} = -i\bar\psi\gamma^\mu\partial_\mu\psi + im\bar\psi\psi, \tag{9}$$

where γ^μ satisfies $\{\gamma^\mu,\gamma^\nu\} = 2g^{\mu\nu}$, and $g^{\mu\nu} = \text{diag}\,(-1,1)$ is the Minkowski metric. We choose $\gamma^0 = i\sigma_y$, $\gamma^1 = \sigma_x$, and $\gamma^{01} = \sigma_z$.

The translation symmetry acts on the low-energy fields by

$$t : \psi(x) \to e^{ik_F a\sigma_z}\psi(x+a) = \psi(x+a), \tag{10}$$

where we have used the fact that $k_F a \in 2\pi\mathbb{Z}$ for integer filling. Note that, while $\psi(x)$ varies very slowly on the scale of l: $\psi(x) \approx \psi(x+l)$, it is not the case on the scale of a: $\psi(x) \not\approx \psi(x+a)$, hence, that $\psi(x)$ could vary on the scale $R \gg l$ and $R < a$.

Although this kind of model might not seem like the system one would normally consider, it has been argued that classifications and the topological properties of such systems are same as the crystalline phases in general [49]. In other words, all other states belonging to the same topological crystalline phase are smoothly connected to the ground state of such models (dubbed as the smooth state in Ref. [49]), and the smooth state can serve as a representative of the whole phase. In the next section, we are going to obtain the effective field theory in this special limit.

A. Topological term for 1D atomic insulators

As discussed above, the effective theory of an atomic insulator is a $(1+1)$D single massive Dirac theory (9). To make contact with the topological crystal picture, we add a spatially dependent mass term

$$\mathcal{L}_m = im_0\bar\psi e^{i\phi(x)\gamma^{01}}\psi, \tag{11}$$

where $\gamma^{01} = \gamma^0\gamma^1$, $m_0 > 0$, and we assume $m \gg m_0$. Here the spatial dependence of the mass term is encoded in the function $\phi(x)$. Similar to the fermion fields, $\phi(x)$ could vary on the scale R. Here we focus on a special configuration of $\phi(x)$ such that it is a monotonic function whose value changes abruptly by 2π at the location of atoms as shown in Fig. 2. It can be shown that these kinds of spatially dependent mass terms trap a charge-1 bound state with a finite energy at the interfaces of $\phi(x)$. These charge-1 bound states are precisely the building blocks in the topological crystal approach and correspond to the physical atoms.[2]

We now discuss the classification of such mass interfaces parametrized by $\phi(x)$. We will show that the mass interfaces are classified by $H^1(B\Gamma,\mathbb{Z})$. To systematically discuss the configurations of $\phi(x)$, we consider the cell decomposition of $\mathbb{R}$ by the FDs. Here each one cell $\Sigma_{1,(i)}$ is simply a unit cell and is labeled by a group element g in the group of discrete translation $\Gamma \cong \mathbb{Z}$. Two neighboring 1-cells $\Sigma_{1,(i)}$, $\Sigma_{1,(j)}$ meet at a single 0-cell $\Sigma_{0,(ij)}$, which is labeled by the generator t of the translation group Γ. This kind of cell decomposition by the FDs applies to any crystalline symmetry.

With this cell decomposition, we can now discuss the configurations of $\phi(x)$ more systematically. We will first focus on the discontinuous configurations of $\phi(x)$ since the general structure can be seen more clearly in this limit. A

[2]More formally, we note that the function $\phi(x)$ defines a map $\phi : X \to \mathfrak{M}_1$, where $\mathfrak{M}_1$ is the space of $(1+1)$D fermionic short-range entangled states with U(1) symmetry. The configuration of $\phi(x)$ we choose gives a noncontractible loop in $\mathfrak{M}_1$ every time we go through a unit cell and the bound state is associated to the winding number $\pi_1(\mathfrak{M}_1) = \mathbb{Z}$.

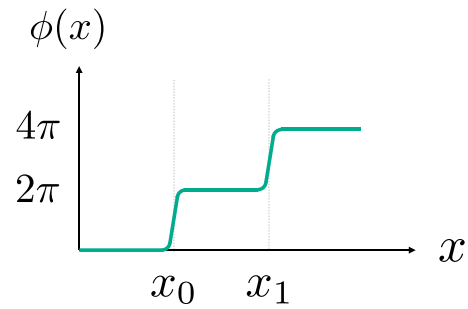

FIG. 2. A typical configuration of the phase $\phi(x)$ of the mass term. $\phi(x)$ jump by 2π at the location of an atom.

discontinuous configuration of $\phi(x)$ is modeled by having a constant function in each 1-cell $\Sigma_{1,(i)}$. At the intersecting 0-cell $\Sigma_{0,(ij)}$, where $\Sigma_{1,(i)}$ and $\Sigma_{1,(j)}$ meet, we have the relation

$$\phi(\Sigma_{1,(j)}) = \phi(\Sigma_{1,(i)}) + 2\pi\tau(\Sigma_{0,(ij)}),\ \ \tau(\Sigma_{0,(ij)}) \in \mathbb{Z}. \quad (12)$$

The integer-valued function τ satisfies

$$\tau(\Sigma_{0,(ij)}) + \tau(\Sigma_{0,(jk)}) = \tau(\Sigma_{0,(ik)}). \quad (13)$$

Moreover, there is a redundancy since, if we modify the configuration of ϕ as

$$\begin{aligned}\phi(\Sigma_{1,(i)}) &\to \phi(\Sigma_{1,(i)}) + 2\pi h(\Sigma_{1,(i)}),\\ \tau(\Sigma_{0,(ij)}) &\to \tau(\Sigma_{0,(ij)}) + h(\Sigma_{1,(j)}) - h(\Sigma_{1,(i)})\end{aligned} \quad (14)$$

with $h(\Sigma_{1,(i)}) \in \mathbb{Z}$, we obtain the same configuration of ϕ, which means that τ is a $\mathbb{Z}$-valued cocycle in $H^1(M, \mathbb{Z})$. This, however, does not mean that $\phi(x)$ is classified by the cellular cohomology $H^1(M, \mathbb{Z})$ of the manifold M, and we are not considering arbitrary interfaces. What we are interested in are the *symmetric deformation classes* of the interface configurations of ϕ with a charge-1 particle at each interface. Taking the typical configuration of $\phi(x)$ shown in Fig. 2 as an example, one can see that all the deformations, which respect the translation symmetry, will not change the 2π jumps at the locations of atoms. This structure can be captured by identifying the integer-valued transition function τ as the pullback $\tau = f^*\alpha$, where $\alpha \in H^1(B\Gamma, \mathbb{Z})$ by the map $f : M \to B\Gamma$. The general construction of the map f is given in Appendix B. In our case the map f is constructed as follows. We note that for each 1-cell $\Sigma_{1,(i)}$, there is a dual 0-cell $\Sigma^\vee_{0,(i)}$. Similarly, for each 0-cell $\Sigma_{0,(ij)}$, there is a dual 1-cell $\Sigma^\vee_{1,(ij)}$. The map f is constructed such that every dual 0-cell $\Sigma^\vee_{0,(i)}$ is mapped to the based point $*$ in $B\Gamma$, and a dual 1-cell $\Sigma^\vee_{1,(ij)}$ is mapped to the nontrivial loop labeled by the generator $t \in \pi_1(B\Gamma) = \mathbb{Z}$:

$$\begin{aligned}&f : M \to B\Gamma,\\ &\Sigma^\vee_{0,(i)} \mapsto *,\\ &\Sigma^\vee_{1,(ij)} \mapsto t \in \pi_1(B\Gamma) = \mathbb{Z}.\end{aligned} \quad (15)$$

As a result, dual 1-cells (or the original 0-cells) are in one-to-one correspondence with the generator t of the translation group Γ. This has a following implication: let x_0 be a point inside a 1-cell, a path connecting x_0 to gx_0 is labeled by a group element $g \in \Gamma$. This property is generally true for any space group G_s: any such path can be labeled by a group element $g \in G_s$.

Since we have $\tau = f^*\alpha$, the redundancy of the mass interfaces (14) is restricted as we now discussed. We recall that $H^1(B\Gamma, \mathbb{Z}) \cong H^1(\Gamma, \mathbb{Z})$ is the quotient of 1-cocycles by 1-coboundaries. The cocycle condition reads as

$$\alpha(g_1) + \alpha(g_2) = \alpha(g_1 g_2). \quad (16)$$

In other words, $\alpha(g)$ is a group homomorphism of Γ. The coboundaries in this case are all trivial:

$$\begin{aligned}&\delta\mu : \Gamma \to \mathbb{Z},\\ &g \mapsto 0.\end{aligned} \quad (17)$$

One can easily see that $H^1(B\Gamma, \mathbb{Z}) = \mathbb{Z}$ with the generator given by $\alpha(t) = 1$ where t is the generator of the translation group Γ. Using our construction of the map f, we have $h(\Sigma_{1,j}) = h(\Sigma_{1,i})$ due to Eq. (17). The only remaining redundancy is given an overall shift by 2π, which will not affect the value of τ, and hence the 2π jumps of $\phi(x)$ at the locations of atoms. This is similar to the redundancy of changing the integer labeling of the atoms. Therefore, the symmetric deformation classes of the interfaces are classified by $H^1(B\Gamma, \mathbb{Z}) = \mathbb{Z}$.

To obtain an effective theory, we couple the fermion to an external background U(1) gauge field A_μ. By integrating out the massive fermion, the effective action contains the following topological term:

$$\begin{aligned}S_{\text{eff}} &= \frac{1}{4\pi}\int \epsilon^{\mu\nu}\phi(x)F_{\mu\nu}d^2x\\ &= \frac{1}{2\pi}\int \epsilon^{\mu\nu}A_\mu\partial_\nu\phi(x)d^2x.\end{aligned} \quad (18)$$

By requiring the effective action to be gauge invariant under $A_\mu \to A_\mu + \partial_\mu\alpha$, we find the current

$$J^\mu = \frac{1}{2\pi}\epsilon^{\mu\nu}\partial_\nu\phi \quad (19)$$

is conserved.

In the limit where $\phi(x)$ is discontinuous, the density is given by

$$\rho = \frac{1}{2\pi}\partial_x\phi = \sum_i \delta(x - x_i), \quad (20)$$

where the discrete nature of the density of an atomic insulator is recovered. Note that, if we define the theory on a finite system with size L, the total charge of the system is

$$Q_{\text{tot}} = \int_0^L \frac{1}{2\pi}\partial_x\phi\, dx = \frac{1}{2\pi}[\phi(L) - \phi(0)] = N. \quad (21)$$

This topological term also reveals the "Thouless pump" response for the atomic insulators [63]. There is a net charge flow through the system when the phase field ϕ winds 2π in time.

In general, there is a coefficient ν in front of the topological term (18). To show this coefficient is quantized, we proceed with the following argument. Consider ϕ is time independent and the spatial dependence is given by Eq. (12) with $\tau = 1$. We then integrate along the x direction and the topological

term becomes

$$\begin{aligned} S_{\text{eff}} &= \frac{\nu}{2\pi}\int \epsilon^{\mu\nu}A_\mu\partial_\nu\phi d^2x \\ &\sim \nu\sum_i \int A_0\delta(x-x_i)d^2x \\ &= \sum_i \nu\int A_0(x_i)dt, \end{aligned} \tag{22}$$

where the gauge transformations of $A_0(x_i)$ can be different for different i. We obtain a sum of $(0+1)$D effective actions, each of which is the effective action of an atom coupled to the U(1) gauge field. By the gauge invariance, we see the ν has to be quantized to integers.

B. Taking the smooth limit

In the previous section, we take the limit where $\phi(x)$ is discontinuous in order to make a clear connection to the building block picture. We also see that these discontinuous configurations of $\phi(x)$ are classified by $\alpha \in H^1(B\Gamma, \mathbb{Z})$. Here we show that it is possible to take a limit where $\phi(x)$ is a smooth function such that $\phi(x)$ is still classified by $H^1(B\Gamma, \mathbb{Z})$. Moreover, we are going to take the limit where $\phi(x)$ is as smooth as possible such that $\partial_x\phi(x)$ is uniform. After taking such smooth limit, we will obtain an effective field theory which works in the usual IR limit, where the correlation length ξ does not have to be much smaller than the unit cell a.

Let us recall that the defining property of an element $\alpha \in H^1(B\Gamma, \mathbb{Z})$ is that the pairing satisfies

$$\int_{C_1} \alpha \in \mathbb{Z}, \tag{23}$$

where C_1 is the nontrivial 1-cycle of $B\Gamma$. We pull this back by using the map $f : M \to B\Gamma$, and the corresponding 1-cocycle $e_1 \in H^1(M, \mathbb{Z})$ satisfies

$$\int_{\Sigma_1^\vee} e_1 = \int_{\Sigma_1^\vee} f^*\alpha \in \mathbb{Z}, \tag{24}$$

where $\Sigma_1^\vee$ is a dual 1-cell (unit cell) in the real space. This integral essentially counts the number of atoms in a unit cell.

We would like to obtain a low-energy effective field theory where all the fields are smooth. At the same time, we want to preserve the classification of $\phi(x)$ given by $H^1(B\Gamma, \mathbb{Z})$. The way to achieve this is to consider closed 1-forms with integral periods.[3] Now we replace the cocycle on the left-hand side of Eq. (24) by a smooth differential 1-form E_1 with integral periods:

$$\int_{\Sigma_1^\vee} E_1 = N_t \in \mathbb{Z}, \tag{25}$$

where $E_1 = d\phi/2\pi$, and ϕ is a smooth function. Then we identify the integer N_t with the right-hand side of Eq. (24):

$$N_t = \int_{\Sigma_1^\vee} f^*\alpha \in \mathbb{Z}. \tag{26}$$

Representatives of the smooth 1-form E_1 can be obtained by solving Eq. (25). We consider a smooth function $\phi(x)$ satisfying

$$\int_{x_0}^{x_0+a} d\phi = [\phi(x_0+a) - \phi(x_0)] = 2\pi\tau, \tag{27}$$

where we have restored the unit-cell size a for the sake of clarity. An example of such function, which is as smooth as possible and satisfying Eq. (27), is given by

$$\phi(x) = \frac{2\pi}{a}\tau x = b_1\tau x, \tag{28}$$

where $b_1 = 2\pi/a$ is the reciprocal lattice vector. (This is essentially the "labeling" field introduced by Haldane [64].) We can then define a smooth 1-form

$$E_1 = \frac{1}{2\pi}\partial_x\phi(x)dx = \frac{1}{2\pi}\tau b_1 dx. \tag{29}$$

This is a closed 1-form with integral period since, if we integrate over a unit cell, we have

$$\int_{\Sigma_1^\vee} E_1 = \int_{x_0}^{x_0+a} \frac{1}{2\pi}\tau b_1 dx = \tau \in \mathbb{Z}, \tag{30}$$

which is the property that we want.

In general, there will be time dependence in ϕ so that we can define the time component of the 1-form $E_0 = \partial_t\phi dt/2\pi$. Written in terms of these smooth 1-form E, we have the following topological term:

$$\int A \wedge E = \frac{1}{2\pi}\int \epsilon^{\mu\nu}A_\mu b_\nu d^2x. \tag{31}$$

We have thus reproduced the effective field theory of an atomic insulator in Refs. [57–61]. As one can see from the above discussion, the 1-form $E = d\phi/2\pi$ basically tells us where to decorate the zero-dimensional (0D) building blocks. Therefore, our approach gives a direct correspondence between the topological terms and the topological crystal picture.

This discussion can be generalized to atomic insulators in higher dimensions. For example, in 2D and 3D, we expect there are topological terms of the form

$$\begin{aligned} S_{\text{eff}} &= \frac{\nu}{2}\int \epsilon_{IJ}A \wedge E^I \wedge E^J, \\ S_{\text{eff}} &= \frac{\nu}{6}\int \epsilon_{IJK}A \wedge E^I \wedge E^J \wedge E^K, \end{aligned} \tag{32}$$

where, for a translation in the Ith direction, E^I is the differential form representative of the cocycle in $H^1(BT_I, \mathbb{Z})$. In Appendix D, we give a detailed derivation of the topological

[3] Recall that a closed k-form ω on M has integral periods if, for every smooth k-cycle C in M, the integral $\int_C \omega$ is an integer. Moreover, a closed k-form ω has integral periods if and only if the de Rham class of ω lies in the image of the change-of-coefficients map

$$H^k(M, \mathbb{Z}) \to H^k(M, \mathbb{R}) \cong H^k_{dR}(M),$$

where $H^k_{dR}(M)$ denotes the de Rham cohomology of M [80]. Loosely speaking, a closed k-form with an integral period serves as a differential form representative of an element in $H^k(M, \mathbb{Z})$.

term (32) for the 2D atomic insulators. Generalizing to 3D atomic insulators is straightforward.

The physical meaning of the topological terms (32) is that there is a charge ν per unit cell as one can see from the effective action of the mass interface obtained by integrating out the spatial directions. Those terms also describe higher-dimensional analogs of the Thouless pump [65,66]. Such kinds of topological terms for atomic insulators are discussed in Ref. [61] in the context of topological elasticity theory (see also Refs. [57–60]), where θ^I fields are interpreted as the phonon fields. Since the topological terms we obtained above take essentially the same form, this suggests that there could be an elasticity interpretation for the spatially dependent mass terms. Indeed, in the case where the spatially dependent mass terms are generated from coupling to lattice deformations, our topological terms are the topological terms in the elasticity theory.

IV. TOPOLOGICAL TERMS OF TOPOLOGICAL CRYSTALLINE INSULATORS WITH POINT-GROUP SYMMETRY

In this section, we are going to discuss various effective field theories for TCIs with point-group symmetries. We will focus on the reflection, C_N rotation, and C_{nv} symmetries for 1D, 2D, and 3D TCIs. The 1D and 2D TCIs that we are going to discuss are built by placing 0D charges at the high-symmetry points, which do not support protected boundary gapless modes. For 3D TCIs, we will consider the second-order topological phases with gapless chiral hinge models, whose building block picture is given by placing 2D IQH states on high-symmetry planes.

A. 1D insulators with reflection symmetry

We now move on to discuss topological crystalline insulators with reflection symmetry in 1D. The symmetry group we focus on is $G = \mathrm{U}(1) \times D_1$, where the reflection group $D_1 \cong \mathbb{Z}_2$. We are going to focus on the phase of which the building block picture is given by placing a 0D state carrying a unit U(1) charge and a trivial irreducible representation of D_1 at the reflection center.

The low-energy theory of this kind of insulator is given by the following massive Dirac theory:

$$\mathcal{L} = -i\bar{\psi}\gamma^\mu \partial_\mu \psi - m_1 \bar{\psi}\gamma^{01}\psi \tag{33}$$

with the reflection symmetry acting on the fermions by

$$g_r : \psi(x,t) \to \gamma_1 \psi(-x,t). \tag{34}$$

We are going to show that this Dirac theory indeed describes the TCI we are interested in. We proceed with the dimensional reduction procedure by adding a spatially varying mass term:

$$\mathcal{L}_m = -im_2 \bar{\psi} e^{i\phi(x)\gamma^{01}} \psi, \tag{35}$$

where we require that $m_1 \gg m_2 > 0$. The reflection symmetry requires that $\phi(x) = \pi - \phi(-x) \mod 2\pi$. The phase $\phi(x)$ could wind nontrivially in space subjecting to the constraint given by the reflection symmetry. If we consider a configuration of $\phi(x)$ such that it winds 2π along a path passing through the reflection center (as shown in Fig. 3), by solving the bound state directly for this mass interface, one can confirm that there is a charge-1 bound state sitting at the reflection center. This is precisely the building block picture for this phase, which justifies the claim that Eq. (33) describes the TCI we are interested in.

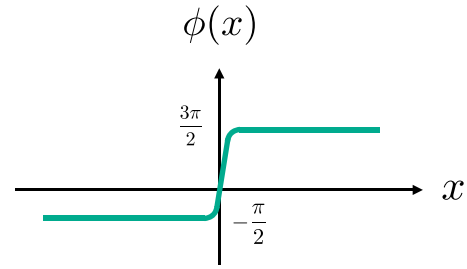

FIG. 3. A typical configuration of $\phi(x)$ which supports a charge-1 bound state at the reflection center.

We are going to show that the mass interfaces parametrized by $\phi(x)$ are classified by the cellular cohomology $H^1(BD_1, \mathbb{Z}^r)$ with a twisting coefficient $\mathbb{Z}^r$, which will be defined below. To proceed, we first discuss the cell decomposition given by the FDs. As shown in Fig. 4, there are two 1-cells $\Sigma_{1,(0)}$, $\Sigma_{1,(1)}$ and a single 0-cell $\Sigma_{0,(01)}$ at the reflection center. The dual-cell structure is also shown in Fig. 4, which contains two dual 0-cells $\Sigma^\vee_{0,(0)}$, $\Sigma^\vee_{0,(1)}$ and one dual 1-cell $\Sigma^\vee_{1,(01)}$. With this choice of cell decomposition, there is a map $f : M \to BD_1$. Written explicitly, the map $f : \Sigma^\vee_{0,(0)} \mapsto *$, $\Sigma^\vee_{0,(1)} \mapsto *$, $\Sigma^\vee_{1,(01)} \mapsto g_r$, where $g_r \in \pi_1(BD_1) \cong D_1$ denotes the nontrivial group element in D_1.

We consider the configurations of $\phi(x)$ such that it is a constant function within the two 1-cells $\Sigma_{1,(0)}$, $\Sigma_{1,(1)}$. At the intersecting 0-cell $\Sigma_{0,(01)}$, the constant functions satisfy the relation

$$\phi(\Sigma_{1,(1)}) = \phi(\Sigma_{1,(0)}) + 2\pi r(\Sigma_{0,(01)}), \tag{36}$$

where $r(\Sigma_{0,(01)}) \in \mathbb{Z}$. The reflection symmetry gives the following condition:

$$\phi(\Sigma_{1,(0)}) + \phi(\Sigma_{1,(1)}) = \pi \mod 2\pi \tag{37}$$

as well as a nontrivial action on the integer-valued function r:

$$g_r r = -r. \tag{38}$$

However, there is a redundancy since, if we modify the configuration of ϕ as

$$\begin{aligned} &\phi(\Sigma_{1,(i)}) \to \phi(\Sigma_{1,(i)}) + 2\pi h(\Sigma_{1,(i)}), \\ &r(\Sigma_{0,(01)}) \to r(\Sigma_{0,(01)}) + h(\Sigma_{1,(1)}) - h(\Sigma_{1,(0)}), \end{aligned} \tag{39}$$

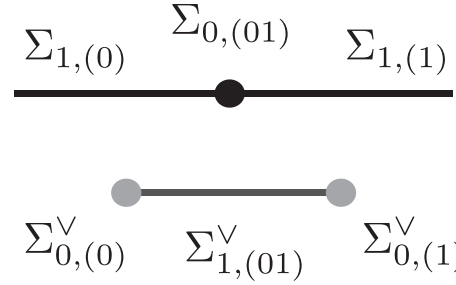

FIG. 4. Reflection-symmetric cell decomposition (above) and the dual-cell decomposition (below).

we obtain the same configuration of $\phi(x)$. These conditions tell us that r is a $\mathbb{Z}$-valued cocycle in $H^1(M,\mathbb{Z}^r)$ with a twisting coefficient given by Eq. (38).

We consider the mass interface such that r is given by the pullback $r = f^*\upsilon$ of $\upsilon \in H^1(BD_1,\mathbb{Z}^r) \cong \mathbb{Z}_2$. To understand this $\mathbb{Z}_2$ classification, we note that the coboundaries in $H^1(BD_1,\mathbb{Z}^r)$ are of the form

$$\begin{aligned} \delta\nu^0 : D_1 &\to \mathbb{Z}, \\ g_r &\mapsto 2m \end{aligned} \tag{40}$$

for some $m \in \mathbb{Z}$, where ν^0 is a function taking the based point $* \in BD_1$ to an integer $\nu^0(*) \in \mathbb{Z}$. By using the map $f : M \to BD_1$, we have

$$\begin{aligned} h(\Sigma_{1,(0)}) &= \nu^0(f(\Sigma_{1,(0)})) = \nu^0(*), \\ h(\Sigma_{1,(1)}) &= \nu^0(f(\Sigma_{1,(1)})) = \nu^0(g_r \cdot *), \end{aligned} \tag{41}$$

where $g \cdot * \sim *$ in the classifying space BD_1. Using Eq. (40), we have $h(\Sigma_{1,(1)}) - h(\Sigma_{1,(0)}) = \delta\nu^0 = 2m$. As a result, there is an equivalence relation $r \sim r + 2m$, and the nontrivial winding of the phase $\phi(x)$ has a $\mathbb{Z}_2$ classification. Pictorially, it is easy to see that an interface with a 4π jump can be deformed into a configuration with no interface while preserving the reflection symmetry.

After coupling to the U(1) gauge fields and integrated out the massive fermions, we obtain a topological term which takes the same form as Eq. (18). The difference is that $\phi(x)$ has to satisfy Eq. (37) due to the reflection symmetry. We thus define a 1-form

$$dP = \frac{d\phi}{2\pi}. \tag{42}$$

The topological term becomes

$$S_{\text{eff}} = k \int A \wedge dP, \tag{43}$$

where the coefficient $k = 1$ in our example. Note that the coefficient k is $\mathbb{Z}_2$ valued since the mass interfaces have $\mathbb{Z}_2$ classification. In the next section, we are going to show how to connect the topological term (43) to the known result in Refs. [59,67] by taking the smooth limit for $\phi(x)$.

1. Smooth limit

Now we would like to consider smooth configurations of $\phi(x)$ such that the mass interfaces are still classified by $H^1(BD_1,\mathbb{Z}^r)$. To proceed, we first rewrite Eq. (36) in terms of the cellular cohomology:

$$\int_{\Sigma_1^\vee} dP_1' = \int_{\partial\Sigma_1^\vee} P_1' = r, \tag{44}$$

where, for the sake of convenience, we have defined $P_1' = \phi/2\pi - 1/4$ to subtract the constant $\pi/2$ contribution in ϕ. P_1' is now simply odd under refection: $g_r : P_1' \to -P_1'$.

What we are looking for is the smooth version of Eq. (44) such that the 1-form dP_1' is constructed by smooth functions. This is achieved by considering the following smooth 1-form with integral periods:

$$\begin{aligned} \int_{-x_0}^{g_r\cdot(-x_0)} d\tilde{P}_1 &= \int_{-x_0}^{x_0} d\tilde{P}_1 \\ &= \tilde{P}_1(x_0) - \tilde{P}_1(-x_0) \\ &= r, \end{aligned} \tag{45}$$

where $|x_0| \gg \xi$ and $\tilde{P}$ is smooth. We can thus write the low-energy effective action in terms of the smooth 1-form $\tilde{P}$:

$$S_{\text{eff}} = k \int A \wedge d\tilde{P}. \tag{46}$$

Under the reflection symmetry $\tilde{P} \to -\tilde{P}$. After an integration by parts, we recognized that Eq. (46) is essentially the effective action obtained in Refs. [59,67], and $\tilde{P}$ can be interpreted as the spatially dependent electric polarization.

B. 2D insulators with rotational symmetry

Here we discuss the topological term of fermionic TCIs with $\mathrm{U}(1) \times C_N$ symmetry.[4] The classification of these systems has been computed in Ref. [68] by using the topological crystal approach. For the sake of simplicity, here we focus on the states with no charge and thermal Hall conductivity, and with a building block picture given by placing a 0D state carrying a unit U(1) charge and a trivial C_N charge at the rotational center.

The low-energy field theory of this state is given by a $(2+1)$D massive Dirac theory:

$$\mathcal{L} = -i\bar{\Psi}\gamma^\mu\partial_\mu\Psi + im_0\bar{\Psi}\sigma_3\Psi, \tag{47}$$

where $\Psi = (\psi_1, \psi_2)$, and σ_i are Pauli matrices in the flavor space. The mass term here guarantees that the Chern number is zero. The C_N rotation acts on the fermions by

$$u : \Psi(\boldsymbol{r}) \to \exp\left(\frac{i}{2}\frac{2\pi}{N}\gamma^0\sigma_3\right)\Psi(R\boldsymbol{r}). \tag{48}$$

One can recover the building block state by adding the following spatially varying mass term:

$$\mathcal{L}_m = im\bar{\Psi}\left[n^1(\boldsymbol{r})\sigma_1 + n^2(\boldsymbol{r})\sigma_2\right]\Psi, \tag{49}$$

where we require that $m_0 \gg m > 0$ and consider the configuration of n^1 and n^2 such that there is a bound state carrying a unit U(1) charge at the origin. An example of such configuration would be a "hedgehog" with a singularity at the origin. Usually, a hedgehog configuration is invariant under a continuous rotational symmetry; here we only require that it is invariant under a discrete C_N rotation. We note that Shiozaki shows there there is an isomorphism between the group of 0D building blocks and the K group of the Dirac Hamiltonians with the hedgehog-mass potential with a unit winding number [69]. Starting from a 0D Hamiltonian describing the 0D building state, one can obtain the massive Dirac theory (47) by using his general construction.

[4]More precisely, the symmetry is $[\mathrm{U}(1) \times C_N]/\mathbb{Z}_2$, as the C_N rotation U defined in Eq. (48) obeys $U^N = (-1)^{N_f}$, where N_f is the total fermion number under U(1).

Since the system is rotational invariant, it is convenient to parametrize the mass term by

$$n^1 = n_r \cos n_\theta,\ n^2 = n_r \sin n_\theta, \tag{50}$$

where n_r can be taken to be a constant almost everywhere and $n_r \to 0$ as $r \to 0$. Following from the C_N transformation on the fermions [Eq. (48)], n_θ must satisfy

$$n_\theta\left(\theta + \frac{2\pi}{N}\right) = n_\theta(\theta) + \frac{2\pi}{N} \bmod 2\pi. \tag{51}$$

In general, the singularity at the origin is described by a 1-form ω_1 such that $d\omega_1 = (\partial_i\partial_j - \partial_j\partial_i)n_\theta \neq 0$. As we will discuss in detail below, this 1-form ω_1 is classified by $H^1(BC_N, \mathbb{Z}_N)$.

After coupling the fermion to a U(1) gauge field and integrate out the massive fermions, the effective theory contains the following topological term:

$$S_{\text{eff}} = \int A \wedge \omega_2, \tag{52}$$

where the 2-form ω_2 is the Euler class in $H^2(M, \mathbb{Z})$. A perturbative derivation of this topological term is given in Appendix E. In general, we have $\omega_2 = n^*\tau_2$, where τ_2 is 2-form in the space of the mass parameters. However, we are going to show that the topological crystal picture tells us that the 2-form ω_2 should be identified with the pullback $f^*\alpha_2$, where $\alpha_2 \in H^2(BC_N, \mathbb{Z})$ and the map $f : M \to BC_N$ is the map from the manifold M to the classifying space BC_N.

The appearance of the Euler class $H^2(M, \mathbb{Z})$ is very natural (see Refs. [53,70] for encountering the Euler class in similar situations). Note that since n^1 and n^2 transform as the regular representation of the C_N rotational symmetry, it makes sense to view them as a vector field $\boldsymbol{n} = (n^1, n^2)$. Formally, we have a $\mathbb{R}^2$ real-vector bundle V over the manifold M (we will always assume the manifold M to be a Euclidean space $\mathbb{E}^2$), and the vector field $\boldsymbol{n}$ is the section of this bundle: $n : M \to V$ such that $\pi \circ n = id$, where π is the projection $\pi : V \to M$. The singular configurations of $\boldsymbol{n}$ correspond to the zero sections of the vector bundle V, and it is well known that the Euler class $e(V) \in H^2(M, \mathbb{Z})$ counts the number of zero sections [71].

Now we discuss how to construct the 2-form ω_2 explicitly. We begin with the cell decomposition of $\mathbb{R}^2$ given by the FDs. Each 2-cell $\Sigma_{2,(i)}$ is labeled by a group element $g \in C_N$. Two neighboring two cells $\Sigma_{2,(i)}$, $\Sigma_{2,(j)}$ meet at a single 1-cell $\Sigma_{1,(ij)}$, which is labeled by the generator $u \in C_N$. There is a unique 0-cell Σ_0 sitting at the rotational center. An example of the C_4-symmetric cell decomposition is shown in Fig. 5(a), and the corresponding dual-cell decomposition is shown in Fig. 5(b).

We now discuss the configurations of the mass term parametrized by Eq. (50) from a more general perspective. Since we only require that the mass term be invariant under a discrete C_N rotation, n_θ can be chosen to be a constant in each 2-cell $\Sigma_{2,(i)}$. At the intersections of 2-cells, n_θ could jump abruptly. We proceed with the following systematic discussion. At the 1-cell $\Sigma_{1,(ij)}$ where $\Sigma_{2,(i)}$ and $\Sigma_{2,(j)}$ meet, we have the relation

$$n_\theta(\Sigma_{2,(j)}) = n_\theta(\Sigma_{2,(i)}) + \frac{2\pi}{N}c(\Sigma_{1,(ij)}),\ c(\Sigma_{1,(ij)}) \in \mathbb{Z}. \tag{53}$$

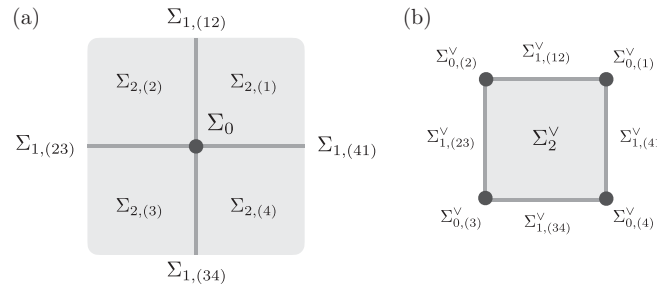

FIG. 5. (a) The cell decomposition for a system with C_4 symmetry, and (b) the corresponding dual-cell decomposition.

A typical configuration of n_θ for C_4-symmetric system is shown in Fig. 6. The integer-valued function c satisfies

$$c(\Sigma_{1,(ij)}) + c(\Sigma_{1,(jk)}) = c(\Sigma_{1,(ik)}). \tag{54}$$

There is a redundancy of the function $c(\Sigma_{1,(ij)})$ since we obtain the same configuration of n_θ after we modify the configuration as

$$\begin{aligned} &n_\theta(\Sigma_{2,(i)}) \to n_\theta(\Sigma_{2,(i)}) + 2\pi h(\Sigma_{2,(i)}),\\ &c(\Sigma_{1,(ij)}) \to c(\Sigma_{1,(ij)}) + h(\Sigma_{2,(j)}) - h(\Sigma_{2,(i)}), \end{aligned} \tag{55}$$

where $h(\Sigma_{2,(i)}) \in \mathbb{Z}$. Formally, c is a $\mathbb{Z}$-valued cocycle in $H^1(M, \mathbb{Z})$. Here we consider the interface such that $c = f^*\alpha_1$, where $\alpha_1 \in H^1(BC_N, \mathbb{Z}_N)$, which is lifted to $C^1(BC_N, \mathbb{Z})$ by the embedding $\mathbb{Z}_N \sim [0, N-1) \subset \mathbb{Z}$. The deformation classes of the n_θ interfaces are classified by $H^1(BC_N, \mathbb{Z}_N) = \mathbb{Z}_N$. If we choose $c(\Sigma_{1,(ij)}) = 1$, we obtain a class of interfaces of n_θ satisfying Eq. (51). Such choice can always be made since we can always choose $\alpha_1(u) = 1$, where u is the generator of the C_N rotation and $\alpha(u) \in H^1(BC_N, \mathbb{Z}_N)$. We then have

$$c(\Sigma_{1,(ij)}) = \alpha_1(f(\Sigma_{1,(ij)})) = \alpha_1(u) = 1, \tag{56}$$

where we have used the fact that $f : \Sigma_{1,(ij)} \mapsto u$ for every 1-cell $\Sigma_{1,(ij)}$.

We now use the cocycle $c \in H^1(M, \mathbb{Z})$ to construct the desired 2-form in the topological term. At the level of cellular cohomology, we would like to have some 2-cocycle $w = \delta c$

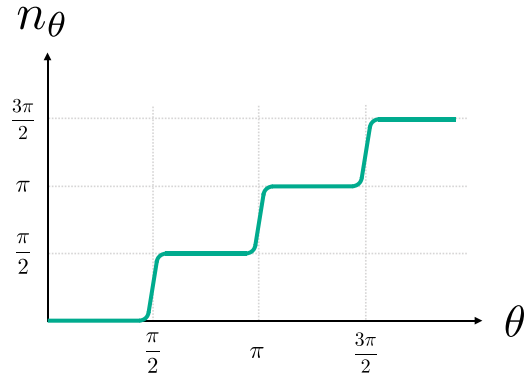

FIG. 6. A typical configuration of n_θ for systems with C_4 symmetry.

satisfying the following property:

$$\frac{1}{N}\int_{\Sigma_2^\vee} w = \frac{1}{N}\int_{\Sigma_2^\vee} \delta c = \frac{1}{N}\int_{\partial\Sigma_2^\vee} c = 1. \tag{57}$$

Physically, this means that n_θ rotates by 2π as it goes around the origin along the 1-cells, which, intuitively, corresponds to having a vortex configuration of $\boldsymbol{n}$ with strength 1. There will be a localized charge-1 bound state trapped at the vortex core, which reproduces the building block picture. We claim the property (57) is satisfied if $\delta c = f^*\delta\alpha_1$. Using Eq. (56), we can explicitly check Eq, (57) is satisfied:

$$\begin{aligned}\frac{1}{N}\int_{\Sigma_2^\vee} w &= \frac{1}{N}\int_{\partial\Sigma_2^\vee} c \\ &= \frac{1}{N}\sum_{i=1}^{N} c(\Sigma_{1,(i,i+1)}) \\ &= \frac{1}{N}\sum_{i=1}^{N} \alpha_1(g) \\ &= 1.\end{aligned} \tag{58}$$

The 2-form ω_2 we are looking for is the differential form representative of the 2-cocycle w, which is a 2-form with integral periods. Now we discuss an explicit construction of the 2-form ω_2. First we need to use two patches U_0 and U_1 to cover the real space $\mathbb{R}^2$ such that the singularity of the section $\boldsymbol{n}$ (at the origin) is contained entirely in U_0, and that U_1 covers $\mathbb{R}^2 - D_0$, where D_0 is the disk covered by U_0. Let $\rho_0(r)$ and $\rho_1(r)$ be the partition of unity satisfying $\rho_0(r) + \rho_1(r) = 1$ subordinate to U_0 and U_1. In the patch U_1, we use the configuration of n_θ discussed above and partition of unity to define a 1-form

$$\omega_1^{(1)} = -\rho_0\frac{dn_\theta}{2\pi} = \rho_0\sum_{i=1}^{N}\frac{c_{i,i+1}}{N}\delta\left(\theta - \frac{2\pi c_{i,i+1}}{N}\right)d\theta, \tag{59}$$

where we have used a shorthand notation $c_{i,j}$ to denote $c(\Sigma_{1,ij})$ and $c_{N,N+1} = c_{N,1}$. In the patch U_0, we define the 1-form $\omega_1^{(0)} = \rho_1 dn_\theta/2\pi$.

Finally, we construct the 2-form

$$\omega_2 = d\omega_1^{(1)} = -\frac{1}{2\pi}d\rho_0 \wedge dn_\theta \tag{60}$$

such that it has an integral period:

$$\int_M \omega_2 = 1. \tag{61}$$

From the property of the partition of unity, ω_2 has support near the intersection $U_0 \cap U_1$. One can show that $d\omega_1^{(0)} = d\omega_1^{(1)}$ so that they piece together to a well-defined 2-form ω_2. We will then drop the superscript when it is not relevant to the context. Equation (61) can be checked explicitly as follows:

$$\begin{aligned}\int_M \omega_2 &= \int_M d\omega_1^{(1)} \\ &= -\frac{1}{2\pi}\int_M d\rho_0 \wedge dn_\theta \\ &= -\frac{1}{2\pi}[\rho_0(\infty) - \rho_0(0)]\int dn_\theta \\ &= \frac{1}{2\pi}\int\sum_{i=1}^{N}\frac{c_{i,i+1}}{N}\delta\left(\theta - \frac{2\pi c_{i,i+1}}{N}\right)d\theta = 1.\end{aligned} \tag{62}$$

The explicit form of the topological term is given by substituting this 2-form $\omega_2 = d\omega_1$ into Eq. (52).

In this example, the coefficient in front of the topological term is 1 by construction. In general, there is a coefficient κ and the topological term takes the form

$$\kappa\int A \wedge d\omega_1. \tag{63}$$

To show that the coefficient κ is quantized, we integrate out the real space. By construction, we have

$$\kappa\int_{M\times S^1} A \wedge d\omega_1 = \kappa\int_{S^1} A_0 dt, \tag{64}$$

which is precisely the effective action of a 0D particle carrying charge κ. Gauge invariance requires that κ is quantized. Moreover, κ is a mod N integer as we now show. From the block equivalence relation in the topological crystal picture, a state with 0 charge is equivalent to a state with N charge at the rotational center. This can be understood as the following deformation process. Starting from a state with no charge, we bring in N additional charge-1 particles to the rotational center while preserving the C_N symmetry [and sending N additional charge-(-1) particles to infinite, which are not relevant to the bulk property]. At the level of field theory, if there are N charge-1 particles at the rotational center, the interface is described by a 2-form $d\omega_1'$, in which $c'_{i,i+1} = N$. However, this 2-form is trivial as one can check as follows:

$$\begin{aligned}\int_M d\omega_1'^{(1)} &= \frac{1}{2\pi}\sum_{i=1}^{N}\frac{c'_{i,i+1}}{N} \\ &= \frac{1}{2\pi}\sum_{i=1}^{N}\frac{c'_{i,i+1} - dh_{i,i+1}}{N} \\ &= 0\end{aligned} \tag{65}$$

where, in the first equality, we have integrated over the r and θ directions, and, in the second equality, we have shifted the cocycle $c'_{i,i+1}$ by a coboundary $dh_{i,i+1} = N$. This implies that κ is a mod N integer.

1. Smooth limit

Here we show that it is possible to deform the function n_θ to a smooth function such that the 2-form ω_2 is smooth almost everywhere except having a singularity at the origin. We begin with the 1-form ω_1. To go to the smooth limit, the key is to consider the smooth 1-form $d\tilde{n}_\theta$ of the angular variable $\tilde{n}_\theta$ such that

$$\begin{aligned}\int_{\Sigma_1^\vee} d\tilde{n}_\theta &= \int_{\theta_0}^{\theta_0+2\pi/N} d\tilde{n}_\theta \\ &= \tilde{n}_\theta\left(\theta_0 + \frac{2\pi}{N}\right) - \tilde{n}_\theta(\theta_0) \\ &= \frac{2\pi}{N}\tilde{c},\end{aligned} \tag{66}$$

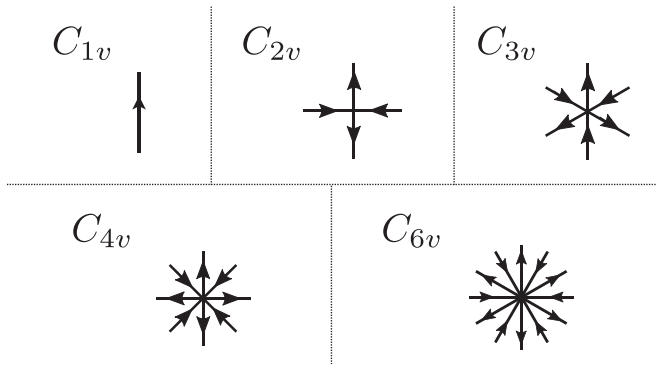

FIG. 7. The top surface view of the 3D topological crystals built from 2D IQH states for C_{nv} point groups. Solid lines represent an IQH state on each mirror plane. The arrows represent the edge chiralities of the IQH states.

where $\tilde{c} \in \mathbb{Z}$ is one-to-one correspondent to $c \in H^1(M, \mathbb{Z})$ in Eq. (53), which is determined by the pullback $f^*\alpha_1$ with $\alpha_1 \in H^1(BC_N, \mathbb{Z}_N)$. The smooth 2-form $\tilde{\omega}_2$ is constructed in same way as in the discontinuous case:

$$\tilde{\omega}_2 = d\tilde{\omega}_1, \tag{67}$$

where $\tilde{\omega}_1 = -\rho_0 d\tilde{n}_\theta/2\pi$ with $\tilde{n}_\theta$ satisfying Eq. (66). Substituting this 2-form into Eq. (63), we obtain the topological term in the smooth limit.

C. 3D topological crystalline insulators

Here we discuss the effective theories of the 3D topological crystalline insulators with $\mathrm{U}(1) \times G_{pg}$, where G_{pg} is a point-group symmetry. The noninteracting classifications have been obtained in Ref. [41] by computing the Atiyah-Hirzebruch spectral sequence for K homology, which is the rigorous mathematical framework of the topological crystal approach for free-fermion systems. We will be focusing on one type of the second-order topological insulators [30,72–74], which break time-reversal symmetry and host protected gapless chiral hinge modes in an open geometry. To illustrate the basic idea, we will consider $G_{pg} = C_{nv}$ for $n = 1, 2, 3, 4, 6$ but our approach can be generalized to other point groups. Such second-order phases can be described by the topological crystal pictures of having some 2D integer quantum Hall (IQH) states placing at some high-symmetry planes. With proper open geometry, the protected chiral hinge modes are directly given by the gapless edge modes of the 2D IQH states [30,74]. It was known that such a type of second-order topological insolators can be well described by the effective axion field proposed in Ref. [62] (see also Ref. [75]). It coincides with the fact that the second-order topological insulators that we considered can be well described by the effective axion field, and the chiral hinge modes are the domain-wall modes between two gapped surface with opposite half quantum anomalous Hall effect [30]. In this section, we will show that the same topological terms can be reproduced by our approach.

The topological crystal states that we are going to focus on are shown in Fig. 7. Those states are obtained by placing a IQH state at each reflection plane with the requirement that all the gapless modes at the rotational axis are gapped out while preserving the symmetry.

It has been shown in Ref. [41] that the bulk of the second-order phases can be described by the following $(3+1)$D massive Dirac theory:

$$\mathcal{L} = -i\bar{\psi}\gamma^\mu\partial_\mu\psi - im_0\bar{\psi}\psi, \tag{68}$$

where we use the following convention for the gamma matrices:

$$\gamma^0 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} = \tau^3,$$
$$\gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix} = i\sigma^i\tau^2,$$
$$\gamma^5 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} = \tau^1. \tag{69}$$

The reflection and the rotation symmetry in the C_{nv} symmetry act on the fermions by

$$g_r^y : \psi(\boldsymbol{r}) \to i\sigma^2\tau^3\psi\left(g_r^y\boldsymbol{r}\right),$$
$$R : \psi(\boldsymbol{r}) \to e^{\frac{i}{2}\theta\sigma^3}\psi(R\boldsymbol{r}). \tag{70}$$

Other reflection symmetries in the C_{nv} group can be generated by the combination of the y reflection g_y and the rotation R.

To connect the massive Dirac theory to the topological crystal states, we add the following spatially dependent mass term:

$$\mathcal{L}_m = -im\bar{\psi}e^{i\phi(\boldsymbol{r})\gamma^5\tau^2}\psi. \tag{71}$$

The reflection and the rotational symmetries act on the phase variable ϕ by

$$g_r^y : \phi(\boldsymbol{r}) \to -\phi\left(g_r^y\boldsymbol{r}\right),$$
$$R : \phi(\boldsymbol{r}) \to \phi(R\boldsymbol{r}). \tag{72}$$

In order for Eq. (71) to be invariant under the symmetry, we must have

$$\phi(\boldsymbol{r}) = -\phi\left(g_r^y\boldsymbol{r}\right) \tag{73}$$

and

$$\phi(\boldsymbol{r}) = \phi(R\boldsymbol{r}). \tag{74}$$

We are going to consider the interface configurations of ϕ such that there is an IQH state at each reflection plane. To simplify the discussion, let us first focus on $G_{pg} = C_{1v}$ in which there is only one reflection symmetry g_r^y. We are going to show that such interfaces of ϕ are classified by $H^1(BC_{1v}, \mathbb{Z}^r)$.

The cell decomposition given by the fundamental domains is the shown in Fig. 8. There are two 3-cells $\Sigma_{3,(0)}$, $\Sigma_{3,(1)}$, and one 2-cell $\Sigma_{2,(01)}$. Similar to the previous discussion, the map $f : M \to BC_{1v}$ maps the dual 0-cells to the based point of BC_{1v}, and it maps the dual 1-cell to the nontrivial loop in BC_{1v} labeled by g_r^y.

We consider the configurations of $\phi(\boldsymbol{r})$ such that it is a constant function within the two 3-cells $\Sigma_{3,(0)}$, $\Sigma_{3,(1)}$. At the intersecting 2-cell $\Sigma_{2,(01)}$, we have the following relation:

$$\phi(\Sigma_{3,(1)}) = \phi(\Sigma_{3,(0)}) + 2\pi r(\Sigma_{2,(01)}), \tag{75}$$

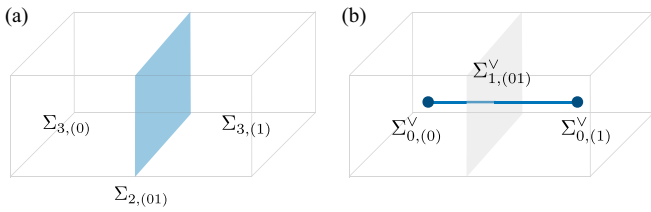

FIG. 8. (a) The cell decomposition for 3D systems with reflection symmetry, and (b) the corresponding dual-cell decomposition.

where $r(\Sigma_{2,(01)}) \in \mathbb{Z}$. The reflection symmetry gives the following condition on ϕ:

$$\phi(\Sigma_{3,(0)}) = -\phi(\Sigma_{3,(1)}). \tag{76}$$

There is also a nontrivial symmetry action on the integer-valued function r:

$$g_r^y r = -r. \tag{77}$$

However, there is a redundancy since, if we modify the configuration of $\phi(\boldsymbol{r})$ as

$$\begin{aligned} \phi(\Sigma_{3,(i)}) &\to \phi(\Sigma_{3,(i)}) + 2\pi h(\Sigma_{3,(i)}), \\ r(\Sigma_{2,(01)}) &\to r(\Sigma_{2,(01)}) + h(\Sigma_{3,(1)}) - h(\Sigma_{3,(0)}), \end{aligned} \tag{78}$$

we obtain the same configuration. From these conditions, we see that r is a $\mathbb{Z}$-valued cocycle in $H^1(M, \mathbb{Z}^r)$ with a twisting coefficient due to the nontrivial action of the reflection (77). A typical configuration of ϕ is shown in Fig. 9. Similar to the discussion in Sec. IV A, we identify r to be the pullback of c: $r = f^*c$, where $c \in H^1(BC_{1v}, \mathbb{Z}^r) \cong \mathbb{Z}_2$. The deformation class of such $\phi(\boldsymbol{r})$ interfaces is classified by $\mathbb{Z}_2$.

With this systematic discussion on the interfaces, we are now ready to discussion the effective field theory. After coupling the fermions to the U(1) gauge field and integrating out the massive fermions, the effective theory contains the following topological term:

$$S = \frac{1}{4\pi} \int AdA \wedge dP, \tag{79}$$

where we have defined $P = \phi/2\pi$. If we consider the nontrivial interface configuration of ϕ given by $r = 1$, it is easy to see that, at the interface, we have

$$S_{\text{Interface}} = \frac{1}{4\pi} \int AdA, \tag{80}$$

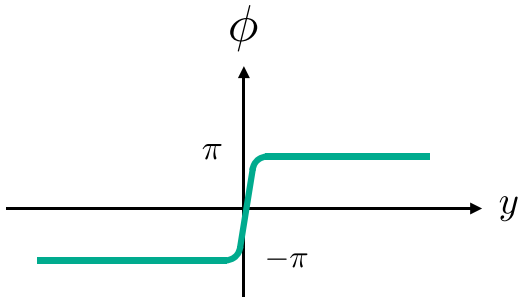

FIG. 9. A typical configuration of $\phi(\boldsymbol{r})$ as a function of y. $\phi(\boldsymbol{r})$ has no spatial variation along the x and z directions.

as we expected that there is an IQH state at the interface. In Ref. [41], the explicit solution of the low-energy states that are localized at the interface is obtained, as well as an effective 2D massive Dirac Hamiltonian that describes an IQH state with a unit Chern number.

1. Smooth limit

To go to the smooth limit, we simply replace the discontinuous 1-form dP by the following smooth 1-form $d\tilde{P}$ with integral periods satisfying

$$\int_{\boldsymbol{r}_0}^{g_r^y \boldsymbol{r}_0} d\tilde{P} = r, \tag{81}$$

where $|\boldsymbol{r}_0|$ is much larger than the correlation length ξ.

The generalization to other C_{nv} symmetry for $n = 2, 3, 4, 6$ is straightforward. In the smooth limit, we have a 1-form $d\tilde{P}^{(n)}$ with integral periods satisfying Eq. (81) and

$$\int_{\boldsymbol{r}_0}^{R\boldsymbol{r}_0} d\tilde{P}^{(n)} = 0. \tag{82}$$

This comes from the requirement that the gapless modes at the rotational axis should be gapped out in order for the IQH states to be glued together. The resulting effective theory is given by

$$S = \frac{1}{4\pi} \int AdA \wedge d\tilde{P}^{(n)}. \tag{83}$$

The above action is essentially the same as the action for effective axion field proposed in Ref. [62], where $\tilde{P}^{(n)}$ serves as the effective axion field. Therefore, our method indeed reproduces the axion effective action for the second-order topological insulators. Moreover, our approach shows that the 1-form $d\tilde{P}^{(n)}$ constructed from the axion field $\tilde{P}^{(n)}$ should be classified by $H^1(BG_{pg}, \mathbb{Z}^r)$ for the second-order topological insulators.

2. Physical responses

For the sake of completeness, we briefly discuss the magnetoelectric responses for the second-order topological insulators governed by $\tilde{P}^{(n)}$. When $\tilde{P}^{(n)}$ is a constant, the integrand of Eq. (83) is a total derivative, and thus Eq. (83) cannot have any response. Therefore, we need certain spatial or temporal dependence in $\tilde{P}^{(n)}$ to get any responses. Here the spatial dependence in $\tilde{P}^{(n)}$ comes from the mass interfaces in the bulk as discussed in the previous section. In particular, we focus on the case where $\tilde{P}^{(n)}$ is smooth, and the space is infinite in order to avoid subtle issues that could appear on the boundary. The responses we discuss below are essentially the same as in Ref. [62].

The general form of the magnetoelectric effect is given by the conserved current

$$J^\mu = \frac{1}{2\pi} \epsilon^{\mu\nu\lambda\delta} \partial_\nu \tilde{P}^{(n)} \partial_\lambda A_\delta. \tag{84}$$

Specifically, when $\tilde{P}^{(n)}$ is static, the electric current can be induced by an applied electric field as

$$J^i = \sigma^{ij} E_j, \tag{85}$$

with the 3D Hall conductivity

$$\sigma^{ij} = \frac{1}{2\pi}\epsilon^{ijk}\partial_k \tilde{P}^{(n)}. \tag{86}$$

We note that the conductivity σ^{ij} is not quantized by itself in general. The quantized quantity is given by

$$\frac{1}{2}\int_{r_0}^{g_r^y r_0} \epsilon_{ijk}\sigma^{jk} dx^i = \frac{1}{2\pi}\int_{r_0}^{g_r^y r_0} \partial_i \tilde{P}^{(n)} dx^i = \frac{1}{2\pi} r, \tag{87}$$

which is quantized in the unit of $e^2/2\pi h$ if we restore the proper unit. When $\tilde{P}^{(n)}$ is dynamic yet homogeneous, the electric current can be induced by an applied magnetic field as

$$J^i = \frac{1}{2\pi}\partial_t \tilde{P}^{(n)} B^i \,. \tag{88}$$

V. DISCUSSION AND OUTLOOK

In this work, we have proposed a general approach to characterize cSPT phases by their response to spatially dependent mass parameters with interface configurations. These mass interfaces implement the dimensional reduction procedure such that the bound states trapped at the interfaces are precisely the building blocks in the topological crystal picture. To illustrate the main idea, we have focused on the TCIs with both U(1) charge conservation and the crystalline symmetry. We have shown that such mass interfaces with codimension k are classified by $H^k(BG_s, \mathbb{Z})$, and discussed the corresponding topological terms generated by integrating out the massive fermions.

One physical correspondence of the spatially dependent mass terms in TCIs is nonhomogeneous lattice distortions or strain [76,77]. In the case when the couplings between electrons and the lattice distortions take the same form as the mass terms in this work, the topological terms will have an interpretation in the elasticity theory. This point of view provides a guiding principle on characterizing TCIs through lattice distortions.

The topological terms discussed in this paper are by no means an exhaustive list. In particular, these terms are incapable of describing the building blocks that transform nontrivially under the crystalline symmetry. It will be desirable to study these kinds of terms in the future and matching with the formal classifications.

When we consider more general topological crystalline phases, it might be the case that there is no local Lagrangian description for the building block of interest. A simple example is given by a weak topological crystalline superconductors protected by the translation symmetry. It can be thought of as a stacking of 1D Kitaev chains. It has been known that the Kitaev chain is characterized by the Arf invariant, which can not be expressed by a local differential form. One can nevertheless apply the dimensional reduction procedure by adding a mass term to a $(2+1)$D Dirac theory with the interface configurations with respect to the translation symmetry. We expect such mass interfaces are classified by $\tau \in H^1(B\mathbb{Z}, \mathbb{Z})$, which can be pullback by the map $f : M \to B\mathbb{Z}$, giving $x = f^*\tau \in H^1(M, \mathbb{Z})$. The result is that there is a $(1+1)$D Dirac theory describing the Kitaev chain at each mass interface. After integrating out the fermions, we can write the topological term in the following schematic form:

$$\int x \cup \mathrm{Arf} \equiv \mathrm{Arf}[\mathrm{PD}(x)], \tag{89}$$

where $\mathrm{PD}(x)$ denotes a collection of codimension-1 submanifolds, which is Poincaré dual to $x = f^*\tau \in H^1(M, \mathbb{Z})$. $\mathrm{Arf}[\mathrm{PD}(x)]$ denotes the Arf invariant defined on the submanifolds $\mathrm{PD}(x)$. The codimension-1 submanifolds $\mathrm{PD}(x)$ are precisely the location of the mass interfaces. These kinds of topological terms have been considered in Ref. [78] from a more formal point of view. Applying our approach also leads to these kinds of topological terms naturally, and it will be interesting to study these kinds of terms more systematically in the future. Finally, we point out that our approach can be applied to noninvertible topological crystalline phases as well, which provides a way to study these phases in the continuous field-theory framework while keeping a clear physical picture.

ACKNOWLEDGMENTS

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APPENDIX A: REVIEW OF THE CELLULAR COHOMOLOGY

Let X be a space with a cell decomposition in terms of CW complexes. A cellular k-chain is a formal linear combination of oriented k cells with integer coefficient $\mathbb{Z}$. These generate an Abelian group $C_k(X, \mathbb{Z})$. The cellular k-cochain is defined to be a map

$$\alpha : C_k(X, \mathbb{Z}) \to A \tag{A1}$$

and these form a group denoted as $C^k(X, A)$. The pairing of a k-cochain $\alpha \in C^k(X, A)$ and a k-cycle $\Gamma \in C_k(X, \mathbb{Z})$ is a map $C^k(X, A) \otimes C_k(X, \mathbb{Z}) \to \mathbb{R}$, which we denote by

$$\int_\Gamma \alpha. \tag{A2}$$

The cellular coboundary map

$$\delta : C^k(X, A) \to C^{k+1}(X, A) \tag{A3}$$

is defined as

$$\int_\Gamma \delta\alpha = \int_{\partial\Gamma} \alpha. \tag{A4}$$

One can show that $\delta^2 = 0$. We denote the kernel of δ as $Z^k(X, A)$, whose elements are cellular k-cocycles, and the image of δ in $Z^k(X, A)$ as $B^k(X, A)$, the group of exact cellular k-cocycles. The kth cellular cohomology of X with coefficients in A is defined as

$$H^k(X, A) = Z^k(X, A)/B^k(X, A). \tag{A5}$$

APPENDIX B: CONSTRUCTION OF THE MAP $f : M \to BG_s$ FOR GENERAL SPACE GROUPS

Here we give a construction of the map $f : M \to BG_s$. We begin by the following cell decomposition of the real space M, which is assumed to be the Euclidean space $\mathbb{E}^d$.

Given a space group G_s, we can partition the Euclidean space $\mathbb{E}^d$ into fundamental domains accordingly. A *fundamental domain* (FD), also known as an *asymmetric unit* (AU) in crystallography, is the smallest simply connected closed part of space from which, by application of all symmetry operations of the space group, the whole of space is filled. Formally, the partition is written as

$$\mathbb{E}^d = \bigcup_{g\in G_s} g\mathcal{F}, \tag{B1}$$

where $\mathcal{F}$ is a fundamental domain and $g\mathcal{F}$ its image under the action of $g \in G_s$. If g is not the identity of space group G_s, then by definition $\mathcal{F}$ and $g\mathcal{F}$ only intersect in their surfaces at most. The choice of fundamental domain is often not unique; a regular choice of fundamental domain for each wallpaper group and 3D space group is available in the International Tables for Crystallography.

This construction gives the Euclidean space $\mathbb{E}^d$ a cell decomposition Σ. For example, in three dimensions, the 3-cells are the individual (nonoverlapping) copies of FDs. The 2-cells lie on faces where two 3-cells meet, with the property that no two distinct points in the same 2-cell are related by symmetry. Similarly, 1-cells are edges where two or more faces meet, and 0-cells are points where edges meet.

The construction of the map $f : M \to BG_s$ is based on the dual-cell decomposition of the one given above. In particular, there is a one-to-one correspondence between k-cells Σ_k and dual $(d-k)$-cells $\Sigma^\vee_{d-k}$ such that they intersect at a single point. Each fundamental domain $\mathcal{F}$ then corresponds to a dual 0-cell $\Sigma^\vee_0$ and is labeled by a group element in G_s. Moreover, a dual 1-cell $\Sigma^\vee_1$ connecting a dual 0-cell $\Sigma^\vee_0$ (associated to $\mathcal{F}$) to $g\Sigma^\vee_0$ (associated to $g\mathcal{F}$) is also labeled by a group element $g \in G_s$. The map f is then constructed such that it maps these dual 0-cells $\Sigma^\vee_0$ to the base point $\{*\}$ in BG_s, and maps a dual 1-cell $\Sigma^\vee_1$ labeled by g to a link in BG_s labeled by the same $g \in \pi_1(BG_s)$ and so on.

APPENDIX C: CLASSIFYING SPACE OF SPACE GROUPS

Let Γ be the translation group in $\mathbb{R}^d$ and P the point group. The d-dimensional space group G_s fits into a short exact sequence

$$1 \to \Gamma \to G \to P \to 1. \tag{C1}$$

In general, G_s is a subgroup of $\mathbb{R}^d \rtimes O(d)$. We can write an element of G_s as (v, P) with $v \in \Gamma$ and $p \in P$.

Following Ref. [79], the classifying space of G_s can be constructed as follows. First we note that the classifying space $B\Gamma$ of Γ is the d-torus $T^d = \mathbb{R}^d/\mathbb{Z}^d$. The point group P has a nontrivial action on $B\Gamma$ by

$$p[v] = [a(p) + pv], \tag{C2}$$

where $[v]$ denotes an element in $B\Gamma$ with the representative $v \in \mathbb{R}^d$, and a is a lift

$$a : P \to \mathbb{R}^d \tag{C3}$$

such that $(a(p), p) \in G_s$. For symmorphic space groups, a can be chosen to be trivial. For nonsymmorphic space groups, a has to be nontrivial. We have the usual point group action on the contractible universal cover EP of the classifying space BP of P. The classifying space BG_s of G_s can be construed as

$$BG_s = B\Gamma \times_P EP, \tag{C4}$$

where $B\Gamma \times_P EP$ denotes the quotient space $(B\Gamma \times EP)/P$. One can show that this space is the same as

$$BG_s = E\Gamma \times_{G_s} EP, \tag{C5}$$

where G_s acts on $E\Gamma = \mathbb{R}^d$ according to the space-group action and on EP by first projecting G_s to P. The space $E\Gamma \times EP$ is the universal cover since it is contractible.

In this paper, we only consider the symmetry group of the from $G = G_s \times G_{\text{int}}$, where G_{int} is the internal symmetry group. Since G_{int} has trivial action on $\mathbb{R}^d$, the classifying space of G splits as

$$BG = BG_s \times BG_{\text{int}}. \tag{C6}$$

APPENDIX D: THE TOPOLOGICAL TERM OF ATOMIC INSULATORS IN TWO DIMENSIONS

Here we consider the topological terms of higher-dimensional atomic insulators. We will illustrate the main idea in two dimensions, and generalization to higher dimensions is straightforward.

The symmetry group of a 2D atomic insulator is $\mathrm{U}(1) \times \Gamma$, where $\Gamma = T_x \times T_y \cong \mathbb{Z}^2$, and the fermion parity is the $\mathbb{Z}_2$ subgroup of U(1). It is known that the general classification of is $\mathbb{Z} \times \mathbb{Z}$. One of the $\mathbb{Z}$ factors is the integer quantum Hall state, which is not our focus. We will focus on the other $\mathbb{Z}$ factor, which is the classification of 2D atomic insulators. The building block picture is having an atom carrying U(1) charges per unit cell. We will focus on the charge-1 case. We assume that we have added the ancillas and performed the coarse graining with respect to the ancilla's lattice. The unit-cell size is much larger than the lattice space of the ancilla's lattice. The minimal low-energy field theory is given by a two-flavor massive Dirac theory:

$$\mathcal{L} = -i\bar{\Psi}\gamma^\mu\partial_\mu\Psi + im_0\bar{\Psi}\sigma_3\Psi, \tag{D1}$$

where $\Psi = (\psi_1, \psi_2)$, and σ^i are Pauli matrices in the flavor space. The mass term here guarantees that there is no Chern number.

To obtain the building block picture, we add the following spatially varying mass term:

$$\mathcal{L} = im\bar{\Psi}(n^1\sigma_1 + n^2\sigma_2)\Psi, \tag{D2}$$

where n^1, n^2 have spatial dependence. Translation symmetries T_x and T_y require that $n^i(\boldsymbol{r}) = n^i(\boldsymbol{r} + \boldsymbol{a})$ for $i = 1, 2$. We would like to choose configurations of n^1 and n^2 such that there is a charge-1 bound state at original lattice site. It turns out that it is enough to consider n^1 depends only on x and n^2 on y.

The conditions on n^1 and n^2 from the translation symmetries become

$$n^1(x) = n^1(x+1),\ n^2(y) = n^2(y+1). \tag{D3}$$

The generic forms of n^1 and n^2 satisfying Eq. (D3) are given by

$$\begin{aligned} n^1(x) &= x - \frac{1}{2\pi}\theta^1(x), \\ n^2(y) &= y - \frac{1}{2\pi}\theta^2(y), \end{aligned} \tag{D4}$$

where $\theta^1(x)$, $\theta^2(y)$ are $\mathbb{R}/2\pi\mathbb{Z}$-valued functions and their values jump by 2π at the location of atoms. In other words, under that translation, we have

$$\begin{aligned} \theta^1(x+1) &= \theta^1(x) + 2\pi N^1,\ N^1 \in \mathbb{Z} \\ \theta^2(y+1) &= \theta^2(y) + 2\pi N^2,\ N^2 \in \mathbb{Z}. \end{aligned} \tag{D5}$$

Equation (D5) implies that the parameter space is a 2-torus $T^2 = S^1 \times S^1$. If we consider the system with periodic boundary condition, we can think of the field θ as a map $\theta : S^1 \times S^1 \to S^1 \times S^1$.

We now discuss the general classification of the interface configurations of θ^1 and θ^2. Let $\Sigma_{2,(x,y)}$ and $\Sigma_{2,(x+1,y)}$ be two neighboring 2-cells that cover the two neighboring unit cells in real space, related by a translation in the x direction and, similarly, $\Sigma_{2,(x,y)}$ and $\Sigma_{2,(x,y+1)}$ are two neighboring 2-cells related by a translation in the y direction. According to Eq. (D5), we have

$$\begin{aligned} \theta^1(\Sigma_{2,(x+1,y)}) &= \theta^1(\Sigma_{2,(x,y)}) + 2\pi N^1(\Sigma_{1,(x+1,x)}), \\ \theta^2(\Sigma_{2,(x,y+1)}) &= \theta^2(\Sigma_{2,(x,y)}) + 2\pi N^2(\Sigma_{1,(y+1,y)}), \end{aligned} \tag{D6}$$

where $N^1 \in \mathbb{Z}$, $N^2 \in \mathbb{Z}$, and $\Sigma_{1,(x+1,x)}$ is the 1-cell where the two neighboring 2-cells $\Sigma_{2,x+1}$ and $\Sigma_{2,x}$ meet, and similarly for $\Sigma_{1,(y+1,y)}$. It is easy to see that N^1 and N^2 satisfy

$$\begin{aligned} N^1(\Sigma_{1,(x_i,x_j)}) + N^1(\Sigma_{1,(x_j,x_k)}) &= N^1(\Sigma_{1,(x_i,x_k)}), \\ N^2(\Sigma_{1,(x_i,x_j)}) + N^2(\Sigma_{1,(x_j,x_k)}) &= N^2(\Sigma_{1,(x_i,x_k)}). \end{aligned} \tag{D7}$$

There is a redundancy since, if we modify the configuration of θ^1 as

$$\begin{aligned} \theta^1(\Sigma_{2,(x_i,x_j)}) &\to \theta^1(\Sigma_{2,(x_i,x_j)}) + 2\pi h^1(\Sigma_{2,(x_i,x_j)}),\ h^1(\Sigma_{2,(x_i,x_j)}) \in \mathbb{Z}, \\ N^1(\Sigma_{1,(x_i+1,x_i)}) &\to N^1(\Sigma_{1,(x_i+1,x_i)}) + h^1(\Sigma_{2,(x_i+1,x_j)}) - h^1(\Sigma_{2,(x_i,x_j)}), \end{aligned} \tag{D8}$$

we obtain the same configuration of θ^1. There is a similar redundancy for N^2 as well. Therefore, we see that N^1 and N^2 are $\mathbb{Z}$-valued cocycles in $H^1(M, \mathbb{Z})$. Moreover, $N^1 = f^*\alpha$ and $N^2 = f^*\beta$ are the pullback of the cocycle $\alpha \in H^1(BT_x, \mathbb{Z})$ and $\beta \in H^1(BT_y, \mathbb{Z})$.

To obtain the effective field theory, we couple Eq. (D1) to a background U(1) gauge field and integrate out the massive Dirac fermions. According to Ref. [66], we have the following topological term:

$$\begin{aligned} S_{\text{eff}} &= \frac{1}{2}\int \epsilon^{\mu\nu\lambda} A_\mu \partial_\nu n^I \partial_\lambda n^J \tau_{2,IJ}(n) d^3x \\ &= \int A \wedge n^* \tau_2, \end{aligned} \tag{D9}$$

where $\tau_2 = \frac{1}{2}\tau_{2,IJ} dn^I \wedge dn^J$ is a 2-form on the parameter space. Here, since our parameter space is a 2-torus T^2 parametrized by θ^I, the 2-form τ_2 should be proportional to the volume form of the 2-torus:

$$\tau_2 = \frac{1}{8\pi^2}\epsilon_{IJ} d\theta^I \wedge d\theta^J. \tag{D10}$$

The topological term becomes

$$S_{\text{eff}} = \frac{1}{8\pi^2}\int \epsilon^{\mu\nu\lambda}\epsilon_{IJ} A_\mu \partial_\nu \theta^I \partial_\lambda \theta^J d^3x. \tag{D11}$$

Requiring that Eq. (D11) be gauge invariant under $A_\mu \to A_\mu + \partial_\mu f$, we find that the following current has to be conserved:

$$J^\mu = \frac{1}{2}\epsilon^{\mu\nu\lambda}\epsilon_{IJ}\partial_\nu \theta^I \partial_\lambda \theta^J. \tag{D12}$$

To gain more intuition, we focus on the charge density

$$\rho = J^0 = \frac{1}{2}\epsilon^{kl}\epsilon_{IJ}\partial_k \theta^I \partial_l \theta^J. \tag{D13}$$

When the interface is discontinuous, we have

$$\rho = \sum_i \delta(x - x_i)\delta(y - y_i). \tag{D14}$$

We thus recover the discrete nature of the charge density of an atomic insulator.

1. Smooth limit

Now we discuss how to take the smooth limit for the θ^I fields. To preserve the information of $H^1(B\Gamma, \mathbb{Z})$, we consider the following smooth 1-forms with integral periods:

$$\begin{aligned} \int_{x_0}^{x_0+1} E^1 dx &= N^1 \in \mathbb{Z}, \\ \int_{y_0}^{y_0+1} E^2 dy &= N^2 \in \mathbb{Z}, \end{aligned} \tag{D15}$$

where we have defined $E^I = d\theta^I/2\pi$. The smooth limit of the 2-form τ_2 then takes the form

$$\tau_2 = \frac{1}{2}\epsilon_{IJ} E^I \wedge E^J. \tag{D16}$$

Written in terms of the smooth differential forms, the effective action becomes

$$S_{\text{eff}} = \frac{1}{2}\int \epsilon_{IJ} A \wedge E^I \wedge E^J. \tag{D17}$$

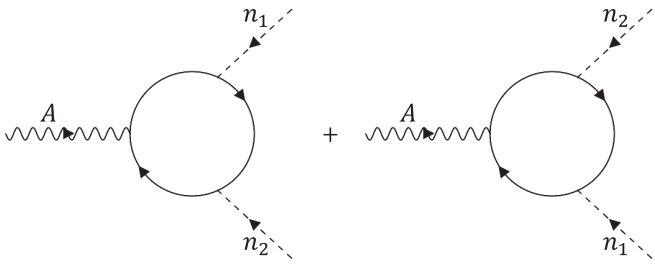

FIG. 10. The Feynman diagrams for Eq. (E5). The solid lines stand for the fermion field.

The simplest configurations of θ^I (and hence E^I) that satisfy Eqs. (D15) and (D15) are given by

$$\theta^1(x) = 2\pi N^1 x = b_1 N^1 x,$$
$$\theta^2(y) = 2\pi N^2 y = b_2 N^2 y, \tag{D18}$$

where b_1 and b_2 are the reciprocal lattice vectors of x and y directions. This discussion can be straightforwardly generalized to higher dimensions.

APPENDIX E: THE TOPOLOGICAL TERM OF ROTATION-INVARIANT INSULATORS IN TWO DIMENSIONS

In this Appendix, we show how to derive the topological term of rotation-invariant insulators in two dimensions by integrating out fermions. We start from the following Lagrangian:

$$\mathcal{L} = i\bar{\psi}\gamma^\mu D_\mu \psi - m_0\bar{\psi}\psi - \bar{\psi} m\boldsymbol{n}\cdot(\gamma^3, -\mathrm{i}\gamma^5)\psi, \tag{E1}$$

where $D_\mu = \partial_\mu + \mathrm{i}A_\mu$, $\boldsymbol{n}(\boldsymbol{r}) = (n^1, n^2) = n_r(\cos n_\theta, \sin n_\theta)$, m_0 is a constant, and the gamma matrices are

$$\gamma^0 = \tau_z\sigma_z\ ,\ \gamma^1 = i\tau_y\sigma_z\ ,\ \gamma^2 = -i\tau_x\sigma_z\ ,\ \gamma^3 = i\tau_0\sigma_y\ ,$$
$$\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3\ . \tag{E2}$$

Here the expressions of the gamma matrices differ from those in the main text by a factor i, but this difference has no influence on the resultant effective field theory.

Performing the Fourier transformation gives the action in the momentum space as

$$S = -\int_k \bar{\psi}_k G^{-1}(k)\psi_k - \int_k\int_q \bar{\psi}_{k+\frac{q}{2}}[A^\mu(q)\gamma_\mu + m\boldsymbol{n}(q)\cdot(\gamma^3, -i\gamma^5)]\psi_{k-\frac{q}{2}}, \tag{E3}$$

where $\mu = 0, 1, 2$, $k = (\omega, \boldsymbol{k})$, $\int_k = \int d^3k/(2\pi)^3$, and $G^{-1}(k) = k_\mu\gamma^\mu + m_0$. Here we use the same Fourier transformation rule for ψ, A, and n as

$$\psi_x = \int_k e^{ikx}\psi_k\ , \tag{E4}$$

and $kx = k_\mu x^\mu$. Integrating out the fermions, the n^1n^2A term is given by the two diagrams in Fig. 10, and reads as

$$\begin{aligned} &- i\int_{k,q_1,q_2} m^2 n^1(q_1)n^2(-q_1-q_2)A_\mu(q_2)(\mathrm{Tr}\,[G(k)\gamma^3 \\ &\quad\times G(k-q_1)\gamma^5 G(k+q_2)\gamma^\mu] + \mathrm{Tr}\,[G(k-q_2)\gamma^5 \\ &\quad\times G(k+q_1)\gamma^3 G(k)\gamma^\mu]) \\ &= -\int_{k,q_1,q_2} m^2 n^1(q_1)n^2(-q_1-q_2)A_\mu(q_2) 8m_0\epsilon^{\mu\nu\rho} \\ &\quad\times \frac{q_{1\nu}q_{2\rho}}{\left(k^2+m_0^2\right)^3} + O(q^3) \\ &= \mathrm{i}\frac{1}{4\pi}\frac{m^2}{m_0^2}\int d^3x\,\epsilon^{\mu\nu\rho}\partial_\nu n_1 n_2 \partial_\rho A_\mu + \cdots . \end{aligned} \tag{E5}$$

Then, the leading-order contribution to the corresponding effective action reads as

$$S_{eff} = -\frac{1}{4\pi}\frac{m^2}{m_0^2}\int d^3x\,\epsilon^{\mu\nu\rho}\partial_\nu n_1\partial_\rho n_2 A_\mu. \tag{E6}$$

Substituting $\boldsymbol{n} = n_r(\cos(n_\theta), \sin(n_\theta))$ and $\kappa = -m^2/(4m_0^2)$ into the equation, we arrive at

$$\frac{\kappa}{2\pi}\int d^3x\,\epsilon^{\mu\nu\rho}A_\mu\partial_\nu n_r^2\partial_\rho n_\theta. \tag{E7}$$

The above expression is Eq. ((63)) with

$$d\omega_1 = \frac{1}{2\pi}\partial_\nu n_r^2\partial_\rho n_\theta dx^\nu\wedge dx^\rho. \tag{E8}$$

The quantization of κ can be derived from Eq. (64).

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