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Theory of interacting topological crystalline insulators

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We study the effect of electron interactions in topological crystalline insulators (TCIs) protected by mirror symmetry, which are realized in the SnTe material class and host multivalley Dirac fermion surface states. We find that interactions reduce the integer classification of noninteracting TCIs in three dimensions, indexed by the mirror Chern number, to a finite group Z_8 . In particular, we explicitly construct a microscopic interaction Hamiltonian to gap eight flavors of Dirac fermions on the TCI surface, while preserving the mirror symmetry. Our construction builds on interacting edge states of $U(1) \times Z_2$ symmetry-protected topological phases of fermions in two dimensions, which we classify. Our work reveals a deep connection between three-dimensional topological phases protected by spatial symmetries and two-dimensional topological phases protected by internal symmetries.

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The prediction and observation of topological crystalline insulators (TCIs) in the SnTe material class has expanded the scope of topological matter and gained wide interest [1–5]. These TCIs possess topological surface states that are protected by mirror symmetry of the rocksalt crystal and become gapped under symmetry-breaking structural distortions [6–9]. These surface states are predicted to exhibit a plethora of novel phenomena ranging from large quantum anomalous Hall conductance [1,10,11] to strain-induced pseudo-Landau levels and superconductivity [12], which are currently under intensive study [13–15].

According to band theory, TCIs protected by mirror symmetry are classified by an integer topological invariant, the mirror Chern number [16]. However, recent theoretical breakthroughs [17–24] have found that the classifications of interacting systems are markedly different from noninteracting systems in various classes of topological insulators and superconductors protected by internal symmetries [25]. This raises the open question about the classification of interacting TCIs protected by spatial symmetries. On the experimental side, a growing body of interaction-driven phenomena has been found in existing TCI materials, including spontaneous surface structural transition and gap generation [6–8] and anomalous bulk band inversion [26]. Moreover, new TCI materials have been predicted in transition-metal oxides [27,28] and heavy fermion compounds [29,30], where strong electron interactions are expected.

Motivated by these theoretical and experimental developments, in this work we study the effect of electron interactions in mirror-symmetric TCIs. Our main result is that interactions reduce the classification of three-dimensional (3D) TCIs from Z in the noninteracting case to Z_8 . We obtain this result by introducing a “domain wall” construction of interacting surface states of 3D TCIs, which exploits the nonlocal nature of mirror symmetry. This construction builds on interacting edge states of two-dimensional (2D) TCIs or $U(1) \times Z_2$ symmetry-protected topological (SPT) phases, which we classify. Our work reveals a deep connection between 3D topological phases protected by spatial symmetries and 2D topological phases protected by internal symmetries.

Interacting TCIs in two dimensions. We first study interacting TCIs in two dimensions to set up the basis of later

analysis in three dimensions. These 2D systems have two independent symmetries: the $U(1)$ charge conservation and the mirror symmetry under the reflection $z \rightarrow -z$, where z is normal to the 2D plane. Since this mirror symmetry is a Z_2 internal symmetry [31], 2D TCIs with mirror symmetry are synonymous to $U(1) \times Z_2$ SPT phases of fermions.

In the absence of interactions, these 2D TCIs are classified by two integers $Z \oplus Z$, the Chern number N and the mirror Chern number n_M associated with occupied bands. Since the Chern number is defined without relying on the mirror symmetry, for our purpose it suffices to consider systems with $N = 0$, for which the mirror Chern number n_M is defined as the Chern number of the occupied bands with the mirror eigenvalue $+1$ [32]. For example, (001) thin films of SnTe and monolayers of IV-VI semiconductors are predicted to be 2D TCIs with $|n_M| = 2$ [33–36].

To study the classification of $U(1) \times Z_2$ SPT phases in the presence of interactions, we follow the general approach presented in the seminal work of Lu and Vishwanath [37] and analyze the stability of noninteracting edge states against interactions. The existence of edge states that can only be gapped by breaking the mirror symmetry signals a 2D SPT phase. To begin with, the low-energy Hamiltonian for edge states of noninteracting TCIs is given by

$$H_0 = \sum_a v_F \int dx (-i\psi_{a,R}^\dagger \partial_x \psi_{a,R} + i\psi_{a,L}^\dagger \partial_x \psi_{a,L}). \quad (1)$$

Here the fermion fields $\psi_{a,R/L}$ denote, respectively, the a th right and left movers ($a = 1, \dots, n$), which transform differently under mirror:

$$M\psi_{a,R}^\dagger M^{-1} = \eta\psi_{a,R}^\dagger, \quad M\psi_{a,L}^\dagger M^{-1} = -\eta\psi_{a,L}^\dagger, \quad (2)$$

where $\eta = \text{sgn}(n_M)$. The difference in mirror eigenvalues forbids single-particle backscattering between left and right movers; hence without interactions, gapless edge states are protected for any integer $n_M \neq 0$. The velocities of different edge modes are chosen to be the same for simplicity; relaxing this condition will not affect any of our conclusions.

We use bosonization to study the effect of interactions at the edge [38,39]. The bosonized Lagrangian for H_0 takes the

form

$$L = \frac{1}{4\pi} K_{ij} \partial_x \phi_i \partial_t \phi_j - \frac{1}{4\pi} v_F (\partial_x \phi_i)^2, \quad (3)$$

where K is an integer-valued matrix given by

$$K = \begin{pmatrix} \mathbf{1}_{n \times n} & 0 \\ 0 & -\mathbf{1}_{n \times n} \end{pmatrix}, \quad (4)$$

with $\mathbf{1}_{n \times n}$ being the $n \times n$ identity matrix. The boson field $\phi_i(x)$ satisfies the Kac-Moody algebra

$$[\phi_i(x), \partial_{x'} \phi_j(x')] = 2\pi i K_{ij}^{-1} \delta(x - x'), \quad (5)$$

and the fermion fields $\psi_{a,R/L}^\dagger$ are given by

$$\psi_{a,R}^\dagger \sim e^{i\phi_a}, \quad \psi_{a,L}^\dagger \sim e^{-i\phi_{n+a}}. \quad (6)$$

Electron interactions such as backscattering and umklapp processes can potentially gap the counterpropagating edge modes. These interaction terms are built from multielectron creation and annihilation operators and are represented by cosine terms of the form $\cos[\Phi_L(x) + \alpha_L(x)]$, where the field $\Phi_L(x) \equiv L^T K \vec{\phi}(x)$ is defined by an integer-valued vector L , and α_L is an arbitrary phase. For our purpose, the interactions must preserve the charge conservation and mirror symmetry indispensable to 2D TCIs. It follows from Eq. (6) that charge conservation requires

$$L^T t = 0, \quad \text{with } t \equiv (\mathbf{1}_n, \mathbf{1}_n)^T, \quad (7)$$

where $\mathbf{1}_n$ is the n -dimensional vector with all components equal to 1. For charge-conserving interactions, we further note the transformation law of the fermion field (2) under mirror symmetry implies

$$M \Phi_L M^{-1} = \Phi_L + \eta \frac{\pi}{2} L^T m, \quad \text{with } m \equiv (\mathbf{1}_n, -\mathbf{1}_n)^T. \quad (8)$$

Hence the condition for mirror symmetry requires

$$L^T m \equiv 0 \pmod{4}. \quad (9)$$

To diagnose SPT phases, we consider sufficiently strong, symmetry-preserving interactions that completely gap the $2n$ edge modes. This can be achieved by adding to the edge Lagrangian (3) n cosine terms [40]:

$$V = \sum_{a=1}^n \lambda_a \cos[\Phi_{L_a}(x)], \quad (10)$$

where different fields Φ_{L_a} are specified by a set of *linearly independent* integer-valued vectors L_a , $a = 1, \dots, n$. To ensure that these fields can simultaneously have classical values, the commutator between any two of them must vanish. Since Eq. (5) implies

$$[\Phi_{L_a}(x), \partial_{x'} \Phi_{L_b}(x')] = 2\pi i L_a^T K L_b \delta(x - x'), \quad (11)$$

this commutativity condition requires

$$L_a^T K L_b = 0, \quad (12)$$

for any indices $a, b = 1, \dots, n$. A set of such vectors $\{L_a\}$ will be referred to as a set of gapping vectors. As a general principle of bulk-boundary correspondence, the symmetry property of gapped edge states due to strong interactions reflects the topological property of the bulk. If the gapped edge preserves

the $U(1) \times Z_2$ symmetry, the bulk is in a trivial phase, i.e., adiabatically connected to an atomic insulator.

We now show this scenario occurs for edge states that have $n = 4$ pairs of counterpropagating modes in the noninteracting limit. Such edge states can be gapped by interactions taking the bosonized form Eq. (10), with the following set of gapping vectors L_a :

$$\begin{aligned} L_1 &= (1, 1, 0, 0; -1, -1, 0, 0)^T, \\ L_2 &= (0, 0, 1, 1; 0, 0, -1, -1)^T, \\ L_3 &= (1, -1, 0, 0; 0, 0, -1, 1)^T, \\ L_4 &= (1, 0, 1, 0; -1, 0, -1, 0)^T. \end{aligned} \quad (13)$$

It is easy to check that L_1, \dots, L_4 satisfy the symmetry conditions (7) and (9), as well as the commutativity condition (12). To motivate the choice of interactions (13), it is useful to regard four edge modes as two pairs of spinful Luttinger liquid in a two-leg fermion ladder system at half-filling. In the absence of interchain tunneling, the left- and right-moving modes have crystal momenta $\pm\pi/2$ and transform oppositely under the lattice translation: $c_R^\dagger \rightarrow i c_R^\dagger$, $c_L^\dagger \rightarrow -i c_L^\dagger$. This is identical to the mirror symmetry transformation property of TCI edge states (2)—the only difference due to the factor i can be eliminated by redefining the symmetry operator [32]. Guided by this correspondence, we choose the interactions for $n = 4$ edge states denoted by L_1 and L_2 to be the bosonized form of the Hubbard interaction in the two-leg ladder, and L_3 and L_4 to be the antiferromagnetic interchain coupling. The former opens up a charge gap and effectively generates two spin chains; the latter opens up a spin gap and leads to a rung-singlet phase that is fully gapped and translationally invariant. Equivalently, the interactions (13) gap the $n = 4$ edge states while preserving the mirror symmetry. A detailed analysis can be found in the Supplemental Material [41]. Therefore, we conclude that a noninteracting 2D TCI with mirror Chern number $n_M = \pm 4$ becomes trivial in the presence of interactions. The additive nature of SPT phases then implies the same conclusion holds for $n_M = 4k$, where k is an integer.

Next we show case by case that the gapped edges of TCIs with $n = 1$ and 2 necessarily break the mirror symmetry spontaneously. First, $n = 1$ edge states consist of a pair of counterpropagating modes, which can be gapped by symmetry-allowed umklapp interactions that backscatter an even number of electrons from left to right movers, described by $\cos(2k\Phi_L)$ with $L = (1, -1)^T$. The gap generation then implies Φ_L is pinned, i.e., $\langle e^{i\Phi_L} \rangle \neq 0$. This signals spontaneous mirror symmetry breaking, as can be seen from (9).

For $n = 2$, by an exhaustive enumeration, we find two types of symmetry-preserving two-body interactions that gap the edge states, which are specified by two sets of gapping vectors $\{L_1, L_2\}$ and $\{L_1, \tilde{L}_2\}$, respectively, with $L_1 = (1, 1; -1, -1)^T$, $L_2 = (1, -1; -1, 1)^T$, and $\tilde{L}_2 = (1, -1; 1, -1)^T$. We further note that the second type of interaction becomes equivalent to the first after redefining the flavor index of the left movers $\psi_{1L}^\dagger \leftrightarrow \psi_{2L}^\dagger$. Hence only the first type of interaction needs to be considered. In terms of the electron

operators, this interaction takes the form

$$V = \lambda_1(\psi_{1R}^\dagger \psi_{2R}^\dagger \psi_{2L} \psi_{1L} + \text{H.c.}) + \lambda_2(\psi_{1R}^\dagger \psi_{2L}^\dagger \psi_{1L} \psi_{2R} + \text{H.c.}). \quad (14)$$

Both terms conserve the number of fermions in each flavor (denoted by $a = 1, 2$) and commute with each other. The first term is an umklapp process that backscatters two electrons with different flavors, and the second term flips the flavor of left and right movers simultaneously. It is convenient to introduce boson fields for each flavor: $\varphi_a = (\phi_{a,R} + \phi_{a,L})/2$ and $\theta_a = (\phi_{a,R} - \phi_{a,L})/2$, with $n_a = \partial_x \theta_a$ being the density of electrons in flavor a . Equation (14) then becomes

$$V = \lambda_1 \cos(2\theta_1 + 2\theta_2) + \lambda_2 \cos(2\theta_1 - 2\theta_2). \quad (15)$$

In the presence of this interaction, the edge becomes gapped when the fields θ_1 and θ_2 are both pinned. This leads to nonzero expectation values of single-particle backscattering operators: $\langle e^{i2\theta_1} \rangle \sim \langle \psi_{1R}^\dagger \psi_{1L} \rangle \neq 0$ and $\langle e^{i2\theta_2} \rangle \sim \langle \psi_{2R}^\dagger \psi_{2L} \rangle \neq 0$, which implies spontaneous mirror symmetry breaking.

The above edge state analysis shows that noninteracting TCIs with mirror Chern number $n_M = \pm 1$ and ± 2 remain topologically nontrivial in the presence of interactions, contrary to the previous case of $n_M = 4k$. Therefore, we conclude that interactions reduce the classification of 2D TCIs protected by mirror symmetry, or $U(1) \times Z_2$ SPT phases, from Z to Z_4 .

In addition to its theoretical value, the above result has important implications for thin films/monolayers of SnTe and other IV-VI semiconductors, which are predicted to be 2D TCIs with $|n_M| = 2$ by band structure calculations [33–36]. Our analysis shows that interactions of the form (14) can qualitatively change the properties of $n = 2$ edge states. At generic filling, only the flavor-flipping λ_2 term is allowed by momentum conservation and it is relevant for repulsive Luttinger interaction from the renormalization group analysis [41]. As a result, there appears a gap in the flavor sector, while the charge sector remains gapless and fluctuates. Boundaries and impurities affect the charge mode by pinning a fluctuating charge density wave, which can be detected by scanning tunneling microscope measurement similar to the case of Luther-Emery liquid with a spin gap [42].

Interacting TCIs in three dimensions. We now turn to TCIs in three dimensions, protected by a single mirror symmetry, say $x \rightarrow -x$. Within band theory, one can define the mirror Chern number n_M on the 2D plane $k_x = 0$ in \mathbf{k} space, which is invariant under this reflection. The integer n_M thus classifies 3D noninteracting TCIs [1,43–45]. The hallmark surface states, present on crystal surfaces symmetric under mirror, consist of $n = |n_M|$ Dirac cones:

$$H_0 = \sum_{a=1}^n v_F \int d\mathbf{r} \psi_a^\dagger(\mathbf{r}) (-i\partial_x s_y + i\partial_y s_x) \psi_a(\mathbf{r}), \quad (16)$$

where $\psi_a^\dagger = (\psi_{a\uparrow}^\dagger, \psi_{a\downarrow}^\dagger)$ is a two-component fermion field. Reflection acts on both the electron's coordinate and spin as follows:

$$M \psi_a^\dagger(x, y) M^{-1} = s_x \psi_a^\dagger(-x, y). \quad (17)$$

The mirror symmetry forbids any Dirac mass term $\psi_a^\dagger s_z \psi_b$, and thus protects these n flavors of gapless Dirac fermions.

Can the above Dirac fermion surface states be gapped by interactions without breaking the charge conservation and mirror symmetry? Finding the answer to this question will hold the key to the classification of interacting TCIs in three dimensions. This is a challenging task requiring a nonperturbative approach to strongly interacting Dirac fermions in two dimensions.

We now demonstrate explicitly that interactions can turn surface states with $n = 8$ flavors of Dirac fermions into a gapped and mirror-symmetric phase without intrinsic topological order (i.e., without fractional excitations). Such a completely trivial surface phase is constructed as follows. First, we introduce a spatially alternating Dirac mass term to H_0 :

$$H_m = \int d\mathbf{r} m(x) \left(\sum_{a=1}^4 \psi_a^\dagger(\mathbf{r}) s_z \psi_a(\mathbf{r}) - \sum_{a=5}^8 \psi_a^\dagger(\mathbf{r}) s_z \psi_a(\mathbf{r}) \right), \quad (18)$$

where $m(x)$ is a periodic function of x that alternates between m_0 and $-m_0$,

$$m(x) = \begin{cases} m_0 & \text{for } (2k-1)L < x < 2kL \\ -m_0 & \text{for } 2kL < x < (2k+1)L. \end{cases} \quad (19)$$

Importantly, the resulting periodic array of Dirac mass domains preserves the mirror symmetry, because $m(x) = -m(-x)$ and $M \psi_a^\dagger(x, y) s_z \psi_a(x, y) M^{-1} = -\psi_a^\dagger(-x, y) s_z \psi_a(-x, y)$.

When the Dirac mass m_0 is large and the width of the domain L is large, the low-energy degrees of freedom are confined to the domain walls at $x = kL$, where the Dirac mass changes sign. As is well known, the mass domain wall of a 2D Dirac fermion hosts a one-dimensional (1D) chiral fermion mode, whose directionality is reversed upon changing the signs of the Dirac masses on both sides. Therefore, our setup described by $H_0 + H_m$ hosts an array of 1D domain wall fermions, one per flavor. On each domain wall, chiral fermions in flavors 1, ..., 4 and those in flavors 5, ..., 8 move in opposite directions, and importantly, have opposite mirror

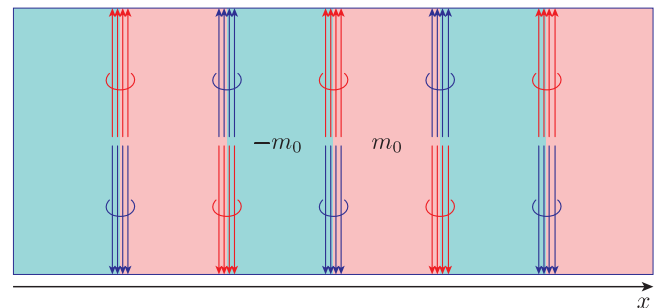


FIG. 1. (Color online) Periodic array of 1D domain wall fermions, generated by spatially alternating Dirac masses to eight flavors of 2D Dirac fermions [see Eqs. (18) and (19)]. 1D chiral fermion modes in flavors 1, ..., 4 (red arrows) and flavors 5, ..., 8 (blue arrows) propagate in opposite directions along a domain wall. Counterpropagating chiral fermions have opposite mirror eigenvalues ± 1 . Each domain wall becomes gapped under the interaction (10), (13), thus leading to a gapped and mirror-symmetric 2D phase.

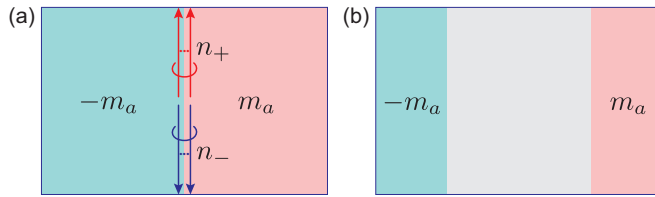


FIG. 2. (Color online) (a) A mass domain wall setup on a 3D TCI surface consisting of n flavors of Dirac fermions. One-dimensional chiral fermions reside at the domain wall at $x = 0$, with n_+ ($n_- = n - n_+$) modes moving in the $+y$ ($-y$) direction, depending on the signs of Dirac masses m_1, \dots, m_n . (b) The domain wall in (a) is expanded to a wide region, sandwiched between semi-infinite regions on the left and on the right, with opposite Dirac masses. Importantly, (a) and (b) are both symmetric under mirror $x \rightarrow -x$ and topologically equivalent. For $n \neq 8k$, the domain wall in (a), hence the middle region in (b) as well, cannot be gapped and mirror symmetric.

eigenvalues ± 1 under the spatial reflection interchanging the two sides of the domain wall, as shown in Fig. 1.

We now draw a connection between the domain wall states on the surface of 3D TCIs to the edge states of 2D TCIs: both are 1D systems of counterpropagating fermions with opposite mirror eigenvalues. Without interactions, the locking between the directionality and mirror eigenvalue forbids single-particle backscattering, leaving such 1D systems gapless. However, as we have shown earlier, the interaction given by Eqs. (10) and (13) opens up a gap when there are four pairs of counterpropagating modes. Applying this interaction to each domain wall that we set up on the surface of noninteracting TCIs then gaps the entire surface state with $n = 8$ Dirac fermions, while preserving the mirror symmetry $x \rightarrow -x$. We have thus explicitly constructed, using a periodic array of domain walls, a completely trivial and gapped surface, the existence of which then implies noninteracting TCIs with mirror Chern number $n_M = 8k$ become trivial in the presence of interactions.

Next, let us consider surface states of TCIs with $n_M \neq 8k$. Below we prove by contradiction that interactions cannot generate a gapped, mirror symmetric and nonfractionalized phase for these surface states [46]. Supposing such a trivial gapped phase exists, it must be adiabatically connectable to a massive Dirac fermion phase, where the Dirac masses are gen-

erated by external mirror symmetry-breaking perturbations. This motivates us to consider a sandwich setup shown in Fig. 2(b), where this trivial phase takes up the region $|x| < L$; to its right is a massive phase with a set of Dirac masses $\{m_a\}$; and to its left the mirror image, a massive phase with opposite Dirac masses $\{-m_a\}$. By construction, this sandwich setup is symmetric under the reflection $x \rightarrow -x$.

We choose L to be much larger than the correlation length of the trivial gapped phase and let the surface Hamiltonian vary slowly with x across the interface at $x = \pm L$, so that the trivial gapped phase (presumed to exist) adiabatically evolves into the massive Dirac fermion phase, without closing gap at the interface. Therefore, the surface is everywhere gapped and as a whole preserves the mirror symmetry.

On the other hand, the sandwich setup is topologically equivalent to a domain wall between two domains with opposite Dirac masses [Fig. 2(a)]. Without interactions, this domain wall hosts $n = |n_M|$ flavors of 1D chiral fermions, with n_+ flavors and n_- flavors moving in opposite directions and carrying opposite mirror eigenvalues. Here n_+ (n_-) is the number of Dirac fermions with $m_a > 0$ ($m_a < 0$), and $n_+ + n_- = n$. Importantly, for $n_+ \neq n_-$, the domain wall must be gapless due to the presence of a net chirality, and for $n_+ = n_- = n/2 \neq 4k$, we have shown earlier that the domain wall cannot be trivially gapped by interactions either. This result of the domain wall contradicts that of the sandwich setup, which is deduced to be gapped under the assumption that a trivial gapped surface is allowed on $n \neq 8k$ TCI surfaces. This contradiction proves the assumption wrong. Instead, 3D TCIs with mirror Chern number $n_M \neq 8k$ cannot have a trivial gapped surface and hence remain topologically nontrivial in the presence of interactions. Putting everything together, we conclude that interactions reduce the classification of 3D TCIs with mirror symmetry from Z to Z_8 .

In addition to reducing the classification of noninteracting TCIs, interactions may also enable new TCI phases that do not exist in free fermion systems, as recently found in other symmetry classes [47,48]. We leave this interesting problem of interaction-enabled TCIs with mirror symmetry for future study.

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