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Anomalous crystal symmetry fractionalization on the surface of topological crystalline insulators

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The surface of a three-dimensional topological electron system often hosts symmetry-protected gapless surface states. With the effect of electron interactions, these surface states can be gapped out without symmetry breaking by a surface topological order, in which the anyon excitations carry anomalous symmetry fractionalization that cannot be realized in a genuine two-dimensional system. We show that for a mirror-symmetry-protected topological crystalline insulator with mirror Chern number $n = 4$, its surface can be gapped out by an anomalous $\mathbb{Z}_2$ topological order, where all anyons carry mirror symmetry fractionalization $M^2 = -1$. The identification of such anomalous crystalline symmetry fractionalization implies that in a two-dimensional $\mathbb{Z}_2$ spin liquid the vison excitation cannot carry $M^2 = -1$ if the spinon carries $M^2 = -1$ or a half-integer spin.

The advent of topological insulators (TIs) [1–3] and topological superconductors (TSCs) [4] has greatly broadened our understanding of topological phases in quantum systems. While the concepts of TIs and TSCs originates from topological band theory of non-interacting electrons/quasiparticles, recent theoretical breakthroughs [5–10] have found that interactions can in principle change fundamental properties of these topological phases dramatically, thus creating a new dimension to explore. In particular, interactions can drive the gapless Dirac fermion surface states of three-dimensional (3D) TIs and TSCs into topologically-ordered phases that are gapped and symmetry-preserving. Nonetheless, such a surface manifests the topological property of the bulk in a subtle but unambiguous way: its anyon excitations have anomalous symmetry transformation properties, which cannot be realized in any two-dimensional (2D) system with the same symmetry.

Given the profound consequences of interactions in TIs and TSCs, the effect of interactions in topological phases protected by spatial symmetries of crystalline solids, commonly referred to as topological crystalline insulators (TCIs) [11], is now gaining wide attention. A wide array of TCI phases with various crystal symmetries have been found in the framework of topological band theory [12, 13]. One class of TCIs has been predicted and observed in the IV-VI semiconductors SnTe, $\mathrm{Pb}_{1-x}\mathrm{Sn}_x\mathrm{Se}$ and $\mathrm{Pb}_{1-x}\mathrm{Sn}_x\mathrm{Te}$ [14–17]. The topological nature of these materials is warranted by a particular mirror symmetry of the underlying rocksalt crystal, and is manifested by the presence of topological surface states on mirror-symmetric crystal faces. Remarkably, there surface states were found to become gapped under structural distortions that break the mirror symmetry [18, 19], confirming the mechanism of crystalline protection unique to TCIs [14].

The study of interacting TCIs has just begun. A recent work by Isobe and Fu [20] shows that in the presence of interactions, the classification of 3D TCIs protected by mirror symmetry (i.e., the SnTe class) reduces from being characterized by an integer known as the mirror Chern number [21] (hereafter denoted by n) to its $\mathbb{Z}_8$ subgroup. This implies that interactions can turn the $n = 8$ surface states, which consists of 8 copies of 2D massless Dirac fermions with the same chirality, into a completely trivial phase that is gapped, mirror-symmetric and without intrinsic topological order. It remains an open question what interactions can do to TCIs with $n \neq 0 \mod 8$. In this work, we take the first step to study strongly interacting TCI surface states for the case $n = 4 \mod 8$.

Our main result is that the surface of a 3D TCI with mirror Chern number $n = 4 \mod 8$ can become a gapped and mirror-symmetric state with $\mathbb{Z}_2$ topological order. Remarkably, the mirror symmetry acts on this state in an anomalous way that all three types of anyons carry fractionalized mirror quantum number $\tilde{M}^2 = -1$ (in this paper we use $\tilde{M}$ to represent the projective representation of mirror symmetry M acting on an anyon), which cannot be realized in a purely 2D system. Furthermore, the anomalous mirror symmetry fractionalization protects a two-fold degeneracy between two mirror-symmetry-related edges. Such anomalous mirror symmetry fractionalization cannot be realized in a 2D system, including a 2D $\mathbb{Z}_2$ spin liquid state [22]. Hence our finding constraints the possible ways of fractionalizing the mirror symmetry in a 2D $\mathbb{Z}_2$ spin liquid [23, 24]. Brief reviews of 3D TCI, 2D $\mathbb{Z}_2$ spin liquids and their edge theory are available in the Supplemental Material [25].

Non-interacting TCIs. We begin by considering non-interacting TCIs protected by the mirror symmetry $x \to -x$. With the mirror symmetry, the extra U(1) symmetry in a TCI does not change the classification in 3D comparing to a mirror protected topological crystalline superconductor. Hence for convenience we choose a TCI as our starting point, although the U(1) symmetry plays no role in this work. As we will explain in Sec. II of the Supplemental Material, in order to produce an anomalous $\mathbb{Z}_2$ surface topological order, the mirror operation must be defined as a $\mathbb{Z}_2$ symmetry with the property $M^2 = 1$. In our previous works on spin-orbit coupled systems, the mirror operation M' acts on electron's spin in addition to its spatial coordinate, which leads to $M'^2 = -1$. Nonetheless, one can redefine the mirror operation by combining M' with the U(1) symmetry of charge conservation $c \to ic$, which restores the property $M^2 = 1$. We note that without the U(1) symmetry only M satisfying $M^2 = +1$ protects nontrivial topological crystalline superconductors.

The mirror TCIs are classified by the mirror Chern number n, defined for single-particle states on the mirror-symmetric plane $k_x = 0$ in the 3D Brillouin zone. The states with mirror eigenvalues 1 and -1 form two different subspaces, each of which has a Chern number denoted by n_+ and n_- respectively. This leads to two independent topological invariants for non-interacting systems with mirror symmetry: the total Chern number $n_T = n_+ + n_-$ and the mirror Chern number $n = n_+ - n_-$.

The TCI with a nontrivial mirror Chern number n has gapless surface states consisting of n copies of massless Dirac fermions, described by the following surface Hamiltonian

$$H_s = v \sum_{A=1}^{n} \psi_A^\dagger (k_x \sigma_y - k_y \sigma_x) \psi_A, \tag{1}$$

where the two-dimensional fermion fields $\psi_A(x, y)$ transforms as the following under mirror operation:

$$M : \psi_A(x, y) \to \sigma_x \psi_A(-x, y). \tag{2}$$

The presence of mirror symmetry (2) forbids any Dirac mass term $\psi_A^\dagger \sigma_z \psi_B$. As a result, the surface states described by (1) cannot be gapped by fermion bilinear terms, for any flavor number n.

We emphasize that the above Dirac fermions on the surface of a 3D TCI cannot be realized in any 2D system with mirror symmetry, as expected for symmetry-protected topological phases in general. According to the Hamiltonian (1), the surface states with $k_x = 0$ within a given mirror subspace are chiral as they all move in the same direction [14]. In contrast, in any 2D system single-particle states within a mirror subspace cannot be chiral (this is demonstrated with a 2D lattice model in Sec. V of the Supplemental Material).

$U(1)$ Higgs phase and Z_2 topological order In this work we study interacting surface states of TCIs with $n = 4$. Starting from four copies of Dirac fermions in the non-interacting limit, we will introduce microscopic interactions and explicitly construct a Z_2 topologically-ordered phase on the TCI surface, which is gapped and mirror symmetric.

Our construction is inspired by the work of Senthil and collaborators [26, 27] on fractionalized insulators. We construct on the surface of a $n = 4$ TCI a Higgs phase with an xy-order parameter $\langle b \rangle \neq 0$, which is odd under the mirror symmetry and gaps the Dirac fermions. Next, we couple these gapped fermions to additional degrees of freedom a_μ that are introduced to mimic a $U(1)$ gauge field. This gauge field a_μ plays three crucial roles: (i) the coupling between matter and a_μ restores the otherwise broken $U(1)$ symmetry, and thus the mirror symmetry along with it; (ii) the Goldstone mode is eaten by the gauge boson and becomes massive; (iii) since the xy-order parameter carries $U(1)$ charge-2, the $U(1)$ gauge group is broken to the $\mathbb{Z}_2$ subgroup in the Higgs phase. Because of these properties, the Higgs phase thus constructed is a gapped and mirror-symmetric phase with $\mathbb{Z}_2$ topological order.

We now elaborate on the construction (details of this construction can be found in Sec. III of the Supplemental Material). First, we relabel the fermion flavors $A = 1, \ldots, 4$ using a spin index $s =\uparrow, \downarrow$ and a $U(1)$-charge index $a = \pm$ (unrelated to the electric charge). We take fermion interactions that are invariant under both the $SU(2)$ spin rotation and the $U(1)$ rotation

$$U(1) : \psi_{as} \to e^{ia\theta} \psi_{as}, \; a = \pm \tag{3}$$

Moreover, we introduce a boson field $b(x, y)$ that carries $U(1)$-charge 2 and is odd under mirror symmetry:

$$U(1) : b \to e^{i2\theta} b, \quad M : b(x, y) \to -b(-x, y), \tag{4}$$

and couple this boson to the massless Dirac fermions as follows

$$H_{bf} = V b^\dagger \psi_{as}^\dagger \tau_{ab}^- \sigma_z \psi_{bs} + \text{h.c.}. \tag{5}$$

When these bosons condense, $\langle b \rangle \neq 0$ spontaneously breaks both the $U(1)$ and mirror symmetry, and gappes out the fermions.

Finally, we introduce another boson vector field $a_\mu(x, y)$, which couples to b and ψ_{as} through minimal coupling. An effective theory of this system has the following form,

$$\begin{aligned} \mathcal{L} = & -i\psi_s^\dagger \alpha^\mu (\partial_\mu + i a_\mu \tau_z) \psi_s + (b \psi_s^\dagger \tau^+ \sigma_z \psi_s + h.c.) \\ & + \frac{1}{2g} |(\partial_\mu - 2ia_\mu) b|^2 + r|b|^2 + u|b|^4 + F_{\mu\nu} F^{\mu\nu}, \end{aligned} \tag{6}$$

where the matrices $\alpha^0 = 1$, $\alpha^x = \sigma_y$ and $\alpha^y = \sigma_x$. Furthermore, we add to the effective action an interation term UN^2, where $N = \psi^\dagger \tau_z \psi + 2b^\dagger b - \nabla \cdot \boldsymbol{E}$ ($E_i = F_{0i} = \partial_0 a_i - \partial_i a_0$ is the electric field strength). In the limit of $U \to \infty$, this enforces the local constraint $N = 0$. As a result, the bare fermion ψ_s and boson b are no longer low energy excitations, since adding them to the ground state violates the constraint $N = 0$ and costs an energy U. Therefore in the low energy effective model ψ_s and b must be screened by the gauge field a_μ and become quasiparticles $\tilde{\psi}_{as} = \psi_{as} e^{ia\theta}$ and $\tilde{b} = b e^{2i\theta}$, where the operator $e^{in\theta}$ creates n gauge charge of a_μ and restores the constraint $N = 0$. In terms of these quasiparticles the effective theory becomes

$$\begin{aligned}\mathcal{L} =& -i\tilde{\psi}_s^\dagger \alpha^\mu (\partial_\mu + i a_\mu \tau_z)\tilde{\psi}_s + (\tilde{b}\tilde{\psi}_s^\dagger \tau^+ \sigma_z \tilde{\psi}_s + h.c.) \\ &+ \frac{1}{2g}|(\partial_\mu - 2ia_\mu)\tilde{b}|^2 + r|\tilde{b}|^2 + u|\tilde{b}|^4 + F_{\mu\nu}F^{\mu\nu},\end{aligned} \tag{7}$$

Furthermore a U(1) gauge symmetry emerges in the low energy Hilbert space defined by the local constraint $N = 0$ [28], Specifically the constraint is the Gauss law and it restricts the low energy Hilbert space to states that are invariant under the gauge transformation

$$U_\phi : \tilde{\psi}_s \to e^{i\phi\tau_z}\tilde{\psi}_s, \quad \tilde{b} \to \tilde{b}e^{2i\phi}, \quad a_\mu \to a_\mu - \partial_\mu \phi. \tag{8}$$

In this effective theory with the emergent U(1) gauge field, condensing the boson $\tilde{b}$ no longer breaks the global U(1) and the mirror symmetries, as it instead breaks the U(1) gauge symmetry to $\mathbb{Z}_2$. Naively the mirror symmetry maps $\langle\tilde{b}\rangle$ to $-\langle\tilde{b}\rangle$. However these two symmetry breaking vacuua are equivalent because they are related by the gauge symmetry transformation $U_{\pi/2} : \tilde{b} \to -\tilde{b}$. This restoration of mirror symmetry becomes clearly manifested if we assume that $\tilde{b}$ and $\tilde{\psi}_s$ transforms projectively under mirror symmetry with the additional U(1) gauge transformation $U_{\pi/2}$,

$$\tilde{M} : \tilde{\psi}_s(r) \to i\tau_z \otimes \sigma_x \tilde{\psi}_s(r'); \tilde{b}(r) \to \tilde{b}(r'). \tag{9}$$

This Higgs phase obtained by condensing charge-2 $\tilde{b}$ field indeed has a $\mathbb{Z}_2$ topological order when the number of Dirac fermions is $n = 4$ [10, 29]. This can be understood by identifying the Bogoliubov quasiparticle $\tilde{\psi}$ and vortices as the anyons e, m, and ϵ (see Sec. II of the Supplemental Material for the definition of the notation) in the $\mathbb{Z}_2$ topological order. $\tilde{\psi}$ becomes the ϵ anyon as both are fermions. As the Higgs field gaps out four Dirac fermions, there are four Majorana fermion, or two complex fermion zero modes in each vortex core. Hence there are two types of vortices, whose core has even or odd fermion parity, respectively. In the case of $n = 4$ it can be shown that the vortices carry Bose statistics (see Sec. IV of the Supplemental Material for the details), and they are mapped to the m and e anyons in the $\mathbb{Z}_2$ topological order, respectively.

Mirror symmetry fractionalization Now we consider how the mirror symmetry acts in the Z_2 spin liquid phase described by Eq. (7). In this effective theory, the $\tilde{\psi}$ field is the fermionic anyon ϵ. Eq. (9) implies that it carries $\tilde{M}^2 = -1$.

Next, we consider how the mirror symmetry acts on the m anyon, which is a vortex of the Higgs field where all core states are empty. Since the mirror symmetry preserves the Higgs field $\langle\tilde{b}\rangle$ but maps x to $-x$, it maps a vortex to an antivortex. Therefore we consider a mirror-symmetric configuration with one vortex and one antivortex, as shown in Fig. 1(a). The symmetry fractionalization of $\tilde{M}^2 = \pm 1$ can be detected from the M parity of the fermion wave function with such a vortice-antivortex pair [30]: for two bosonic vortices, the mirror parity equals to $\tilde{M}^2$.

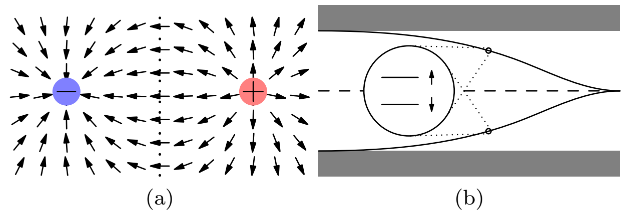

FIG. 1. (a) A vortex and an antivortex. The direction of the arrow represents the phase of the Higgs field $\langle\tilde{b}\rangle$. The doted line is the mirror axis. (b) Illustration of the fermion spectrum flow from the left to the right as we create a vortex-antivortex pair from the vacuum and move them far apart. In this process four vortex core states are separated from the bulk spectrum, two from the conducting band and two from the valence band, and become degenerate zero modes. As illustrated in the inset, the core states are two-fold degenerate with spin $s = \pm 1$.

From Eq. (7) we get the fermion Hamiltonian

$$H = v\tilde{\psi}_s^\dagger (k_x\sigma_y - k_y\sigma_x)\tilde{\psi}_s + \tilde{\psi}_s^\dagger(\langle\tilde{b}\rangle\tau^+ + \langle\tilde{b}\rangle^*\tau^-)\sigma_z\tilde{\psi}_s. \tag{10}$$

It has a particle-hole symmetry $\Xi : \tilde{\psi} \to \sigma_z\tilde{\psi}$ which mapps H to $\Xi H \Xi = -H$. This implies that its spectrum is symmetric with respect to zero. Assume that the dimension of the whole Hilbert space is $4N$, there are $2N$ states with positive energy and $2N$ states with negative energy. For the vortex configuration in Fig. 1(a), there are four complex zero modes, two from each vortex core, which are all unoccupied. Therefore excluding these four states there are $2N-2$ states with negative energy, which are all occupied in the fermion wave function.

Next, we consider the mirror eigenvalues of these $2N-2$ occupied fermion states. Since $\tilde{\psi}$ carries $\tilde{M}^2 = -1$, each state has mirror eigenvalue $\lambda_M = \pm i$. Because both H, Ξ and M are diagonal in pseudospin $s =\uparrow, \downarrow$, all occupied states are pseudospin doublets, and two states in each doublet have the same λ_M. Hence the mirror eigenvalue of all occupied states, organized as $N-1$ doublets, is $(-1)^{N-1} = -1$. Therefore the wave function of two empty vortices is odd under mirror symmetry, which implies that the e particle has the symmetry fractionalization $\tilde{M}^2 = -1$. Combining the results that both e and ϵ carry $\tilde{M}^2 = -1$, we conclude that m anyon also has $\tilde{M}^2 = -1$ (see the discussion in Sec. II of the Supplemental Material).

In summary, the gapped $\mathbb{Z}_2$ surface state we constructed has an anomalous mirror symmetry fractionalization that both types of anyons carry $\tilde{M}^2 = -1$, which cannot be realized in a genuine 2D system. For comparison, it is shown in Sec. II of the Supplemental Material that applying the same construction to a 2D lattice model results in a $\mathbb{Z}_2$ phase with a different mirror symmetry fractionalization which is not anomalous.

Mirror anomaly. The anomalous crystal symmetry fractionalization presented in the surface topological order implies a symmetry protected topological degeneracy associated with the edges of the surface topological ordered region. This mirror anomaly is a remnant of the anomalous surface fermion modes in the free fermion limit. To see this, we consider the setup presented in Fig. 2, in which the Z_2 surface topologically ordered state is terminated at two edges symmetric with respect to the mirror plane, by two regions with opposite $\langle b\rangle = \pm 1$ on either side of the mirror plane, respectively.

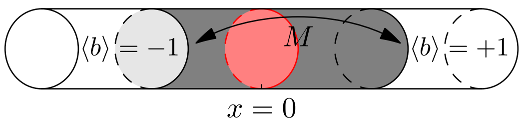

FIG. 2. Two mirror-symmetric edges of a $\mathbb{Z}_2$ surface topological order. The mirror symmetry maps x to $-x$ with respect to the mirror plane marked by the red disk at $x = 0$. The surface topological order, marked by the shade, terminates at edges against two ordered regions with $\langle b\rangle = \pm 1$, respectively.

This setup itself does not break the mirror symmetry, and all local excitations can be gapped everywhere on the surface. Particularly since the $\mathbb{Z}_2$ topological order is not chiral, its edge can be gapped out by condensing either e or m anyons on the edge [31]. The edges next to an ordered phase with $\langle b\rangle \neq 0$ are e-edges, as condensing e breaks the global U(1) symmetry. A $\mathbb{Z}_2$ spin liquid state on a infinite cylinder has four degenerate ground states $|\Psi_a\rangle$, each has one type of anyon flux $a = 1, e, m, \epsilon$ going through the cylinder. On a finite cylinder with two e-edges, only $|\Psi_1\rangle$ and $|\Psi_e\rangle$ remain degenerate, because adding an m or ϵ anyon on the edge costs a finite energy. In a generic $\mathbb{Z}_2$ state this degeneracy can be further lifted by tunneling an e anyon between the two edges, $H_t = \lambda e_L^\dagger e_R^\dagger + \text{h. c.}$, where $e_{L,R}^\dagger$ creates two e anyons on the two edges, respectively. However, the e anyon carries $\tilde{M}^2 = -1$, therefore the tunneling term H_t is odd under mirror and thus forbidden by M. As a result, this two-fold topological degeneracy is protected by the mirror symmetry even in the limit of $L \to 0$. This argument is formulated using the effective edge Lagrangian in the Supplemental Material.

In the limit of $L \to 0$, this topological degeneracy becomes a local degeneracy protected by the mirror symmetry. Therefore if the $\mathbb{Z}_2$ topological order is killed by collapsing two gapped edges, the ground state is either gapless or mirror-symmetry-breaking, and this cannot be avoided regardless of edge types because all types of anyons have $\tilde{M}^2 = -1$. This topological degeneracy reveals the anomalous nature of this mirror symmetry fractionalization. Furthermore, if we collapse two gapless edges of the $\mathbb{Z}_2$ state, the edges remain gapless because the anyon tunneling is forbidden by M. Hence we get a gapless domain wall with central charge $c = 1 + 1 = 2$, which recovers the edge with four chiral fermion modes in the aforementioned free fermion limit. This is explained in more details in Sec. VI of the Supplemental Material.

Conclusion. In this work we show that the surface of a 3D mirror TCI with mirror Chern number $n = 4$, containing four gapless Dirac fermion modes in the free limit, can be gapped out without breaking the mirror symmetry by a $\mathbb{Z}_2$ topological order. This surface $\mathbb{Z}_2$ topological order has an anomalous mirror symmetry fractionalization in which all three types of anyons carry fractionalized mirror symmetry quantum number $\tilde{M}^2 = -1$, and such a topological order cannot be realized in a purely 2D system.

Our finding also puts constraints on possible ways to fractionalize the mirror symmetry in a 2D $\mathbb{Z}_2$ quantum spin liquid [24, 32]. The result of this work indicates that the combination that both the e and m carry the fractionalized $\tilde{M}^2 = -1$ is anomalous and cannot be realized in a 2D $\mathbb{Z}_2$ spin liquid. Furthermore, our result can be easily generalized to also rule out the combination that the e anyon carries spin-$\frac{1}{2}$ and m anyon carries $\tilde{M}^2 = -1$ [33], because if e carries $\tilde{M}^2 = +1$ we can define a new mirror symmetry $M' = Me^{i\pi S^z}$, for which both e and m carries $(\tilde{M}')^2 = -1$ and therefore this combination is also anomalous. In summary, our finding implies that the vison must carry $\tilde{M}^2 = +1$ in a $\mathbb{Z}_2$ spin liquid where the spinon carries a half-integer spin.

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