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Symmetry-protected topological Hopf insulator and its generalizations

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We study a class of $3d$ and $4d$ topological insulators whose topological nature is characterized by the Hopf map and its generalizations. We identify the symmetry $\mathcal{C}'$, a generalized particle-hole symmetry that gives the Hopf insulator a $\mathbb{Z}_2$ classification. The $4d$ analog of the Hopf insulator with symmetry $\mathcal{C}'$ has the same $\mathbb{Z}_2$ classification. The minimal models for the $3d$ and $4d$ Hopf insulator can be heuristically viewed as "Chern insulator $\rtimes S^1$" and "Chern insulator $\rtimes T^2$" respectively. We also discuss the relation between the Hopf insulator and the Weyl semimetals, which points toward a direction for its possible experimental realization.

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The 10-fold-way classification has provided us the prototypes of topological insulators and topological superconductors [1–3]. The usual wisdom is that even the topological insulators with symmetries beyond the 10-fold-way classification can also be understood as these prototypes enriched with other symmetries. Depending on the dimension and symmetry, the boundary states of all these prototypes should be a gapless Dirac fermion, Weyl fermion, or Majorana fermion. One important open question is whether these prototypes represent all possible topological insulators or can we still find exceptions that are different from states in the 10-fold-way classification. In this Rapid Communication, we present a class of such examples, which we generally call Hopf insulators.

The Hopf insulator was studied in Refs. [4,5], but the key symmetry that protects the Hopf insulator was not identified. Without a proper symmetry, the Hopf insulator is actually trivial, which we will explain later in this paper. We demonstrate that the topological nature of the $3d$ Hopf insulator state, previously described only by the homotopy group $\pi_3[S^2] = Z$ in the simplest two-band model [4,5], is more generally given by $\pi_3[\mathrm{Sp}(2N)/\mathrm{U}(N)] = Z_2$ in a multiband model [6], which is the key to stabilizing this state under physical conditions. As long as the system has the translation and a $\mathcal{C}'$ particle-hole symmetry (to be defined later), this Hopf insulator has a $\mathbb{Z}_2$ classification. The same symmetry $\mathcal{C}'$ also gives us a $4d$ topological insulator based on the homotopy group $\pi_4[S^2] = Z_2$ and $\pi_4[\mathrm{Sp}(2N)/\mathrm{U}(N)] = Z_2$.

The minimal model of the Hopf insulator was constructed in Refs. [4,5], but one has to study it with caution. The Brillouin zone of a $3d$ lattice model is a three-torus T^3. A topologically nontrivial mapping from T^3 to S^2 is equivalent to the mapping from S^3 to S^2 (i.e., the so-called Hopf map), as long as any two-torus submanifold of the Brillouin zone has zero winding on the target manifold S^2. Thus, the simplest Hopf insulator Hamiltonian is a two-band model in the $3d$ Brillouin zone, which is the composition of the standard mapping from T^3 to S^3 with winding number 1 and the Hopf map [4,5]

$$H(\mathbf{k}) = \vec{n}(\mathbf{k}) \cdot \vec{\sigma}. \quad (1)$$

The three-component vector field $\vec{n}(\mathbf{k})$ is a mapping from the Brillouin zone to the target space S^2, and we choose it to have Hopf number $+1$. The schematic configuration of $\vec{n}$ in the momentum space is depicted in Fig. 1.

We can introduce the standard CP^1 field $z(\mathbf{k}) = [z_1(\mathbf{k}),\ z_2(\mathbf{k})]^t$ for the three-component vector $\vec{n}(\mathbf{k})$:

$$\vec{n}(\mathbf{k}) = z^\dagger(\mathbf{k})\vec{\sigma} z(\mathbf{k}), \quad (2)$$

and the spectrum of the Hamiltonian is

$$E(\mathbf{k}) = \pm|\vec{n}(\mathbf{k})| = \pm|z(\mathbf{k})|^2 = \pm|\vec{N}(\mathbf{k})|^2, \quad (3)$$

where $\vec{N}(\mathbf{k})$ is a four-component vector defined as $z_1(\mathbf{k}) = N_1(\mathbf{k}) + iN_2(\mathbf{k})$, $z_2 = N_3(\mathbf{k}) + iN_4(\mathbf{k})$. Thus, as long as the length of $\vec{N}$ never vanishes in the Brillouin zone, this system is an insulator with a band gap between the two bands. The configuration of $\vec{n}(\mathbf{k})$ with Hopf number $+1$ corresponds to the configuration of $\vec{N}(\mathbf{k})$ with the winding number $+1$:

$$\text{Hopf number} = \frac{1}{\Omega_3}\int d^3k\ \hat{N}^a \partial_{k_x} \hat{N}^b \partial_{k_y} \hat{N}^c \partial_{k_z} \hat{N}^d, \quad (4)$$

where $\hat{N}(\mathbf{k}) = \vec{N}(\mathbf{k})/|\vec{N}(\mathbf{k})|$ and Ω_3 is the volume of S^3.

As an example of a Hopf insulator, we can choose the following configuration of $\vec{N}(\mathbf{k})$:

$$N_1(\mathbf{k}) = \sin(k_x), \quad N_2(\mathbf{k}) = \sin(k_y), \quad N_3(\mathbf{k}) = \sin(k_z),$$
$$N_4(\mathbf{k}) = m - \cos(k_x) - \cos(k_y) - \cos(k_z), \quad (5)$$

where the Hopf number defined in Eq. (4) equals $+1$ when $1 < m < 3$. This model is essentially the same model constructed in Refs. [4,5]. This two-band model alone appears to be a nontrivial topological insulator with stable edge states. The existence of edge states was demonstrated numerically in Refs. [4,5], and it was shown that the edge state (at least on one of the edges) of this model is a Fermi ring.

The boundary Fermi ring can be heuristically understood as follows: We can parametrize the $3d$ momentum space as (k_r,θ,k_z), where $k_r = \sqrt{k_x^2 + k_y^2}$ and $\tan\theta = k_y/k_x$. Figure 1 shows that every half-plane (k_r,k_z) with fixed θ, $\vec{n}(\mathbf{k})$ has a configuration with Skyrmion number $+1$; thus for every θ with $0 < \theta < 2\pi$, there is a gapless edge state along the radial k_r direction at the XY boundary. These edge states together will form a Fermi ring on the XY boundary. This observation is confirmed by our direct numerical calculation; see Fig. 2. In fact, the Hopf mapping corresponds to the configuration of $\vec{n}$ in the $3d$ Brillouin zone such that the domain wall between $n_3 > 0$ and $n_3 < 0$ forms a torus, and the two-component vector (n_1,n_2) has a nontrivial winding around both directions of the torus. So in this sense, we can call the $3d$ Hopf insulator

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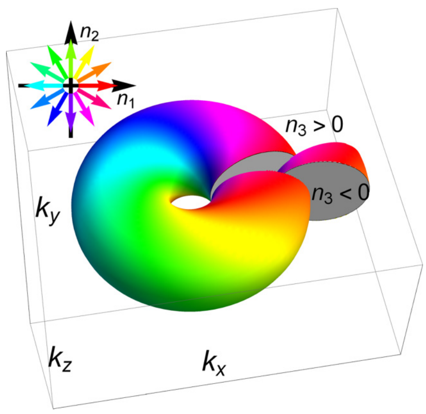

FIG. 1. An illustration of the Hopf map in the momentum space, which is equivalent to T^3. The domain wall $n_3 = 0$ forms a two-torus T^2, and (n_1,n_2) winds around both directions of the torus. Thus intuitively the Hopf insulator can be viewed as Chern insulator $\rtimes$ S^1. The symbol $\rtimes$ represents the 'winding of the Chern insulator along S^1.

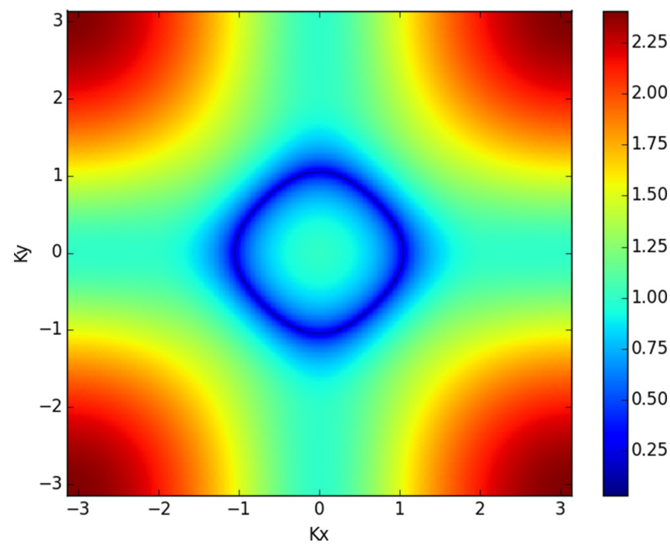

FIG. 2. The Fermi ring at the XY boundary of the minimal two-band model of the Hopf insulator for $m = 2$ in Eq. (5).

Chern insulator $\rtimes S^1$, where $\rtimes$ represents the winding of (n_1,n_2) along S^1, so the Hopf insulator is not a simple direct product between the Chern insulator and S^1. This heuristic picture was previously discussed in Ref. [7].[1]

However, this simple two-band Hopf insulator, without any symmetry, is unstable against mixing with other bands. A generic band insulator consists of m empty bands and n filled bands, and in $\mathbf{k}$ space can be described by an $(m+n) \times (m+n)$ Hermitian matrix $H(\mathbf{k})$. For each value of $\mathbf{k}$, $H(\mathbf{k})$ has m positive eigenvalues, corresponding to the m empty bands, and n negative eigenvalues, corresponding to the n filled bands. Without closing the gap, the m positive eigenvalues (n negative eigenvalues) can all be continuously deformed to $+1$ (-1). Therefore, $H(\mathbf{k})$ takes the form $H(\mathbf{k}) = U(\mathbf{k}) I_{m,n} U^\dagger(\mathbf{k})$, where $I_{m,n}$ is an $(m+n) \times (m+n)$ diagonal matrix with m $+1$'s and n -1's on the diagonal, and $U(\mathbf{k}) \in \mathrm{U}(m+n)$. When there is no symmetry other than the $U(1)$ charge conservation and momentum conservation, the configuration space of the Hamiltonian is topologically equivalent to the complex Grassmannian manifold $\mathrm{Gr}(n,m+n) = \frac{\mathrm{U}(m+n)}{\mathrm{U}(m)\times\mathrm{U}(n)}$ [4]. The band insulator is a map from the Brillouin zone T^d to $\mathrm{Gr}(n,m+n)$, which is induced by classes of mappings $S^d \to \mathrm{Gr}(n,m+n)$ [8,9]; we shall focus on the latter.

In general, $\pi_3[\mathrm{Gr}(n,n+m)] = 0$, as long as n and m do not both equal 1. This observation implies that once the two-band model described above starts mixing with other bands, there will be no nontrivial topological insulator. But in the following we will prove that with a special symmetry $\mathcal{C}'$, this system always has an even number of bands, and its Hamiltonian belongs to the manifold $\mathcal{M} = \mathrm{Sp}(2N)/\mathrm{U}(N)$, and because $\pi_3[\mathrm{Sp}(2N)/\mathrm{U}(N)] = Z_2$ for $N > 1$, the Hopf insulator has $\mathbb{Z}_2$ classification with symmetry $\mathcal{C}'$.

For a $2N$-band system, the symmetry $\mathcal{C}'$ acts on fermion operators as $\mathcal{C}' f_k \mathcal{C}'^{-1} = J f_k^\dagger$. J is a $2N \times 2N$ matrix which we choose to be

$$J = \begin{pmatrix} 0 & I_{N\times N} \\ -I_{N\times N} & 0 \end{pmatrix}. \tag{6}$$

Thus $\mathcal{C}'$ is a generalized particle-hole transformation, and it can be viewed as the product between a particle-hole transformation $\mathcal{C}$ (with $\mathcal{C}^2 = -1$) and the spatial inversion $\mathcal{I}$. The system does not have to satisfy $\mathcal{C}$ or $\mathcal{I}$ individually, and in fact in our model both are explicitly broken. The symmetry $\mathcal{C}'$ implies that for all $\mathbf{k}$, the Hamiltonian $H(\mathbf{k})$ must satisfy

$$J^{-1} H(\mathbf{k}) J = -H(\mathbf{k})^*. \tag{7}$$

Equation (7) implies that for each $\mathbf{k}$, $H(\mathbf{k})$ is in the Lie algebra of $\mathrm{Sp}(2N)$, and there is always an even number of bands. When diagonalized, $H(\mathbf{k})$ takes the form

$$H(\mathbf{k}) = \mathrm{diag}(\lambda_1(\mathbf{k}), -\lambda_1(\mathbf{k}), \ldots, \lambda_N(\mathbf{k}), -\lambda_N(\mathbf{k})). \tag{8}$$

We can continuously deform all of the positive eigenvalues to $+1$ and all of the negative eigenvalues to -1. Therefore, the deformed $H(\mathbf{k})$ takes the form

$$H(\mathbf{k}) = U(\mathbf{k}) I_{N,N} U^\dagger(\mathbf{k}), \tag{9}$$

where $U(\mathbf{k}) \in \mathrm{Sp}(2N)$. We now show that the entire configuration space of the Hamiltonian is $\mathrm{Sp}(2N)/\mathrm{U}(N)$. A generic element that does not move $I_{N,N}$ is $g = \mathrm{diag}(U_1(\mathbf{k}),U_2(\mathbf{k}))$, where $U_1(\mathbf{k}),U_2(\mathbf{k}) \in \mathrm{U}(N)$. However, in order for g to be in $\mathrm{Sp}(2N)$, it has to satisfy

$$\begin{pmatrix} U_1 & \\ & U_2 \end{pmatrix} J \begin{pmatrix} U_1 & \\ & U_2 \end{pmatrix}^T = J. \tag{10}$$

Imposing this condition tells us that $U_1 U_2^T = 1$, which implies that the configuration space of the Hamiltonian is $\mathrm{Sp}(2N)/\mathrm{U}(N)$. From the mathematics

[1] But we would also like to point out that this heuristic picture may not apply for all Hopf insulators, because a half-plane in the Brillouin zone is in principle not periodic; hence a Skyrmion may not be well defined on a half-plane in the Brillouin zone.

literature [10],

$$\pi_3[\mathrm{Sp}(2N)/\mathrm{U}(N)] = \begin{cases} Z & N = 1 \quad (11a) \\ Z_2 & N \geqslant 2 \quad (11b) \end{cases},$$

$$\pi_4[\mathrm{Sp}(2N)/\mathrm{U}(N)] = Z_2. \quad (11c)$$

To connect the two-band Hopf insulator with Hopf number 1 to the nontrivial $2N$-band model, one simply needs to make the Hamiltonian a block-diagonal Hamiltonian, with two bands being the Hopf insulator and the other bands being a $2(N-1)$ band trivial insulator, i.e.,

$$H_{2N\text{-band}}(\mathbf{k}) = \begin{pmatrix} H(\mathbf{k})_{2\times 2} & \\ & I_{N-1,N-1} \end{pmatrix}, \quad (12)$$

where $H(\mathbf{k})_{2\times 2}$ is defined in Eq. (1). In other words, the $U(\mathbf{k})$ matrix in Eq. (9) is also block diagonal, i.e.,

$$U_{2N\text{-band}}(\mathbf{k}) = \begin{pmatrix} U(\mathbf{k})_{2\times 2} & \\ & I_{(2N-2)\times(2N-2)} \end{pmatrix}. \quad (13)$$

Here $U(\mathbf{k})_{2\times 2}$ is a SU(2) matrix that will contribute $n_w = 1$, and $H(\mathbf{k}) = U(\mathbf{k})_{2\times 2}\sigma^3 U(\mathbf{k})^\dagger_{2\times 2}$.

The conclusion that the classification for the multiband system with the $\mathcal{C}'$ symmetry is no larger than $\mathbb{Z}_2$ can be understood as follows. Let us take $N = 2$. The nontrivial mapping from S^3 to Sp(4)/U(2) is induced by the mapping from S^3 to Sp(4), characterized by the winding number $n_w = \frac{1}{24\pi^2}\int d^3k\ \mathrm{tr}[(U^{-1}dU)^3]$, where $U \in \mathrm{Sp}(4)$. Any two $U(\mathbf{k})$ with the same n_w can be continuously deformed into each other, since there is no topological obstruction. In the case of $n_w = 2$, the induced four-band Hamiltonian $H(\mathbf{k}) = U(\mathbf{k})I_{2,2}U^\dagger(\mathbf{k})$ can be continuously deformed into two copies of two-band Hopf insulators, each with the Hamiltonian Eq. (1), whose three-component vectors are $\vec{n}(\mathbf{k})_1$ and $\vec{n}(\mathbf{k})_2$, respectively, where $\vec{n}(\mathbf{k})_1 = -\vec{n}(\mathbf{k})_2$. This is because if $H(\mathbf{k})_1 = \vec{n}(\mathbf{k})_1 \cdot \vec{\sigma}$ is generated by SU(2) matrix $U(\mathbf{k})$, then $H(\mathbf{k})_2 = -H(\mathbf{k})_1$ can be generated by another SU(2) matrix $\tilde{U}(\mathbf{k}) = U(\mathbf{k})i\sigma^2$, which always gives the same n_w as $U(\mathbf{k})$. Then each (k_r,k_z) half-plane for a fixed θ now has zero total Skyrmion number (the Skyrmion numbers of $\vec{n}_1$ and $\vec{n}_2$ cancel out), so this state is a trivial insulator.

The classification for $\mathcal{C}'$ can be understood in another way. Under ordinary $\mathcal{C}$ transformation, the position variables are invariant, but all of the momenta variables pick up a sign. However, under the $\mathcal{C}'$ transformation, the momenta do not change, but all of the position variables pick up a sign. Therefore, for all intents and purposes, we can replace $\mathcal{C}'$ with $\mathcal{C}$ as long as we reverse the roles of the position and momenta variables. Therefore, following Ref. [11], the classification of a d-dimensional topological insulator (TI) with $\mathcal{C}'$ is the same as the classification of a $\delta = 0 - d \equiv 8 - d (\mathrm{mod}\ 8)$-dimensional TI with $\mathcal{C}$, which is simply class C. As expected, the classifications match for all d.

We note that because the general multiband model of the Hopf insulator requires the $\mathcal{C}'$ symmetry which involves spatial inversion, the boundary of the system necessarily breaks $\mathcal{C}'$ and hence the system does not have protected edge states. However, the classification of the Hopf insulator is still well defined in the bulk, like all the topological insulator and superconductors with the ordinary inversion symmetry [12–14].

This heuristic picture of the Hopf insulator in Fig. 1 points toward a possible direction of its experimental realization. The Hopf insulator can be naively viewed as layers of Chern insulators stacked along a ring in the momentum space (with a nontrivial winding along the ring) [7]. A $3d$ Weyl semimetal [15] can be viewed as layers of Chern insulators stacked along a line in the momentum space, and the Chern insulator terminates at the momentum layers with the Weyl points. Now if we can take a Weyl semimetal with two pairs of Weyl points in the momentum space, such as the material $MoTe_2$ [16], and annihilate the Weyl points to connect the Chern lines into a ring, then this system could effectively become a Hopf insulator, with a proper winding of the Hamiltonian along the ring. Its boundary Fermi rings are just connected Fermi arcs of the Weyl semimetal.

Now let us move on to the $4d$ model. A $4d$ band structure is not just for pure theoretical interest; we can also view the fourth momentum as a periodic time coordinate. Thus, the entire band structure can be viewed as a time-dependent $3d$ Hamiltonian. In $4d$, the set of maps $S^4 \to \mathrm{Gr}(n,m+n)$ is classified by $\pi_4[\mathrm{Gr}(n,m+n)]$. We will start with the minimal model $m = n = 1$. In this case, the band insulator is a map $S^4 \to S^2$, which has homotopy group $\pi_4[S^2] = Z_2$.

We need to construct a nontrivial map $F : T^4 \to S^2$. Heuristically, this mapping can be viewed as the following: In the $4d$ space, the domain wall between $n_3 > 0$ and $n_3 < 0$ will form a three-torus T^3, and (n_1,n_2) winds nontrivially along all three directions of the three-torus. Thus, the $4d$ Hopf insulator constructed with the three-component vector $\vec{n}$ and Pauli matrices can be heuristically viewed as Chern insulator $\rtimes T^2$. Consequently, the $3d$ boundary states will have a torus of zero-energy modes (no symmetry is needed in this minimal two-band model).

A concrete band structure of this kind was discussed in Ref. [17]. We review the idea but implement it somewhat differently and also generalize it. F can be constructed via the reduced suspension technique in algebraic topology [18,19]. Pictorially,

$$T^4 \xrightarrow{\Sigma[f]} \Sigma S^2 = S^3 \xrightarrow{f} S^2,$$

where $\Sigma[f]$ [20] is the reduced suspension of the Hopf map f, defined as

$$\Sigma f : (\mathbf{k},t) \mapsto (N_1,\ N_2,\ N_3,\ N_4), \quad (14)$$

where $\vec{N}$ is a four-component vector with nonzero norm:

$$\begin{aligned} N_1 &= \sin(t/2)[\sin k_x \sin k_z \\ &\quad + \sin k_y(m - \cos k_x - \cos k_y - \cos k_z)], \\ N_2 &= \sin(t/2)[\sin k_x(m - \cos k_x - \cos k_y - \cos k_z) \\ &\quad - \sin k_y \sin k_z], \\ N_3 &= \cos t(\sin^2 k_x + \sin^2 k_y) + \sin^2 k_z \\ &\quad + (m - \cos k_x - \cos k_y - \cos k_z)^2, \\ N_4 &= \sin t((m - \cos k_x - \cos k_y - \cos k_z)^2 + \sin^2 k_z). \quad (15) \end{aligned}$$

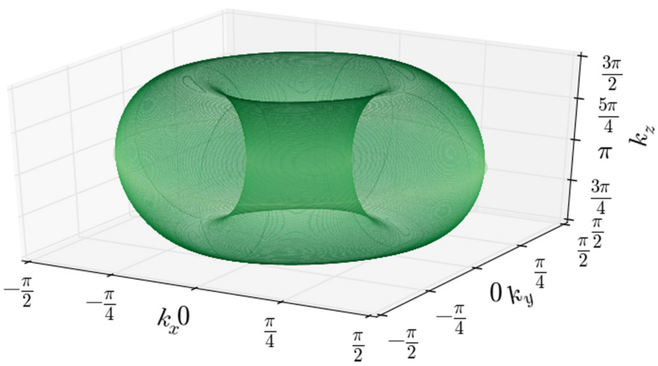

FIG. 3. The boundary zero-energy states of the $4d$ minimal two-band model for Hopf insulator with $m = 2$ in Eq. (15), plotted in the $3d$ boundary Brillouin zone. Because this model can be heuristically viewed as Chern insulator $\rtimes T^2$, its boundary has a torus of zero-energy states.

The Hopf map, as before, is defined as $f : (N_1,N_2,N_3,N_4) \mapsto (n_1,n_2,n_3)$,

$$\begin{aligned} n_1(\mathbf{k},t,m) &= 2(N_1N_3 + N_2N_4), \\ n_2(\mathbf{k},t,m) &= 2(N_1N_4 - N_2N_3), \\ n_3(\mathbf{k},t,m) &= N_1^2 + N_2^2 - N_3^2 - N_4^2. \end{aligned} \tag{16}$$

Finally, we define the Hamiltonian $H(\mathbf{k},t,m)$ (up to normalization) as $H(\mathbf{k},t,m) = \vec{n}(\mathbf{k},t,m) \cdot \vec{\sigma}$. The variable t in this $4d$ model can be viewed as time. This means we can consider our system as an adiabatic time-dependent band insulator, with a period of 2π. In Fig. 3, we plot the zero-energy states computed numerically at the boundary Brillouin zone of the minimal two-band model of the $4d$ Hopf insulator. The zero-energy states indeed form a torus in the boundary Brillouin zone, which is consistent with our expectation.

We now consider a general multiband system and impose the $\mathcal{C}'$ symmetry. With the $\mathcal{C}'$ symmetry, there is still an even number of bands, and just like the $3d$ story discussed before, since $\pi_4[\mathrm{Sp}(N)/\mathrm{U}(N)] = Z_2$ for all N, there is only one class of nontrivial Hopf insulator with the $\mathcal{C}'$ symmetry.

In $4d$ there is a well-known integer quantum Hall state without assuming any symmetry other than the charge conservation [21], but unlike the $2d$ Chern-insulator, the $4d$ integer quantum Hall state necessarily breaks the $\mathcal{C}'$, because its response to the external electromagnetic field $j^e_\mu \sim \epsilon_{\mu\nu\rho\tau\sigma} F_{\nu\rho} F_{\tau\sigma}$ breaks $\mathcal{C}'$, where j^e_μ is the charge current.

In summary, we found a class of $3d$ and $4d$ topological insulators whose topological nature is characterized by the Hopf map and its generalizations. We identified a $\mathcal{C}'$ symmetry which gives these states a $\mathbb{Z}_2$ classification. The states we constructed are also mathematically equivalent to topological superconductors with total spin S_z conservation (but there is no charge conservation). Now the $\mathcal{C}'$ symmetry becomes a special inversion symmetry $\mathcal{I}'$, which is a product of the ordinary inversion and spin S_z flipping. Thus our system can also be viewed as a crystalline topological superconductor with the S_z conservation and the $\mathcal{I}'$ symmetry.

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