Symmetry Protected Topological Hopf Insulator and its Generalizations

Chunxiao Liu,1 Farzan Vafa,1 and Cenke Xu1

1Department of physics, University of California, Santa Barbara, CA 93106, USA

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 isomorphism class $C'$, a generalization of the particle-hole symmetry that gives the Hopf insulator a $Z_2$ classification. The 4d analogue of the Hopf insulator with symmetry $C'$ has the same $Z_2$ classification. The minimal models for the 3d and 4d Hopf insulator can be heuristically viewed as “Chern-insulator $\times S^1$” and “Chern-insulator $\times T^2$” respectively. We also discuss the relation between the Hopf insulator and the Weyl semimetals, which points the direction for its possible experimental realization.

PACS numbers:

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, or Weyl fermion, or Majorana fermion. One important open question is, can 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 paper we present a class of such examples, which we generally call Hopf insulator.

The Hopf insulator was studied in Ref. 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 $\pi_3[Sp(2N)/U(N)] = Z_2$ in a multi-band model [6], which is the key to stabilizing this state under physical conditions. As long as the system has the translation and a $C'$ particle-hole symmetry (to be defined later), this Hopf insulator has a $Z_2$ classification. The same symmetry $C'$ also gives us a 4d topological insulator based on the homotopy group $\pi_4(S^2) = Z_2$ and $\pi_4[Sp(2N)/U(N)] = Z_2$.

The minimal model of the Hopf insulator was constructed in Ref. [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 the target manifold $S^2$ has zero winding on any two-torus submanifold of the Brillouin zone. This Hopf map can be induced from the standard mapping from $T^3$ to $S^3$ with winding number 1. Thus the simplest Hopf insulator Hamiltonian is a two-band model in the 3d Brillouin zone [4, 5]:

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

The three component vector field $\vec{n}(k)$ 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.

FIG. 1: An illustration of the Hopf map in the momentum space. The domain wall $n_3 = 0$ forms a solid torus, and $(n_1, n_2)$ winds around both directions of the torus. Thus intuitively the Hopf insulator can be viewed as “Chern-insulator $\times S^1$”. The symbol $\times$ represents the “winding of the Chern-insulator” along $S^1$.

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

$$ \vec{n}(k) = z^t(k) \vec{\sigma} z(k), $$

the spectrum of the Hamiltonian is

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

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

Thus the simplest Hopf insulator Hamiltonian is a two-band model in the 3d Brillouin zone [4, 5]:

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

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, or Weyl fermion, or Majorana fermion. One important open question is, can 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 paper we present a class of such examples, which we generally call Hopf insulator.

The Hopf insulator was studied in Ref. [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 $\pi_3[Sp(2N)/U(N)] = Z_2$ in a multi-band model [6], which is the key to stabilizing this state under physical conditions. As long as the system has the translation and a $C'$ particle-hole symmetry (to be defined later), this Hopf insulator has a $Z_2$ classification. The same symmetry $C'$ also gives us a 4d topological insulator based on the homotopy group $\pi_4(S^2) = Z_2$ and $\pi_4[Sp(2N)/U(N)] = Z_2$.

The minimal model of the Hopf insulator was constructed in Ref. [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 the target manifold $S^2$ has zero winding on any two-torus submanifold of the Brillouin zone. This Hopf map can be induced from the standard mapping from $T^3$ to $S^3$ with winding number 1. Thus the simplest Hopf insulator Hamiltonian is a two-band model in the 3d Brillouin zone [4, 5]:

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

The three component vector field $\vec{n}(k)$ 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.

FIG. 1: An illustration of the Hopf map in the momentum space. The domain wall $n_3 = 0$ forms a solid torus, and $(n_1, n_2)$ winds around both directions of the torus. Thus intuitively the Hopf insulator can be viewed as “Chern-insulator $\times S^1$”. The symbol $\times$ represents the “winding of the Chern-insulator” along $S^1$.

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

$$ \vec{n}(k) = z^t(k) \vec{\sigma} z(k), $$

the spectrum of the Hamiltonian is

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

FIG. 2: The Fermi ring at the boundary of the minimal two-band model of the Hopf insulator for $m = 2$ in Eq. [5].
where \( \vec{N}(\mathbf{k}) \) is a four component vector defined as \( z_1(\mathbf{k}) = N_1(\mathbf{k}) + i N_2(\mathbf{k}), \quad z_2 = N_3(\mathbf{k}) + i N_4(\mathbf{k}). \) 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:

\[
\text{Hopf number} = \frac{1}{\Omega_3} \int d^3k \: \vec{N}^a \partial_{k_x} \vec{N}^b \partial_{k_y} \vec{N}^c \partial_{k_z} \vec{N}^d, \tag{4}
\]

where \( \vec{N}(\mathbf{k}) = \vec{N}(\mathbf{k})/|\vec{N}(\mathbf{k})| \), and \( \Omega_3 \) is the volume of \( S^3 \).

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

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

the Hopf number defined in Eq. 4 equals +1 when \( 1 < m < 3 \). This model is essentially the same model constructed in Ref. [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 Ref. [4] [5] and it was shown that the edge state of this model is a “Fermi ring”.

The boundary Fermi ring can be heuristically understood as follows: We can parameterize the 3d momentum space as \( (k_x, \theta, k_z) \), where \( k_x = \sqrt{k_x^2 + k_y^2} \), and \( \tan \theta = k_y/k_x \). Fig. 1 shows that for every half plane \( (k_x, k_z) \) with fixed \( \theta \), \( \vec{n}(\mathbf{k}) \) has a configuration with Skyrmion number +1, thus for every \( \theta \) with \( 0 < \theta < 2\pi \), there is a gapless edge state along the radial \( k_x \) direction at the \( (0, 0, 1) \) boundary. These edge states together will form a Fermi ring on the \( (0, 0, 1) \) 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 as “Chern-insulator \( \times S^1 \)”, where \( \times \) 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 \( S^1 \).

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 \( k \) 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 \( H(\mathbf{k}) = U(\mathbf{k}) I_{m,n} U^T(\mathbf{k}) \), 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 \( U(\mathbf{k}) \in U(m+n) \). 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 \( Gr(n, m+n) = U(m+n)/U(m) \times U(n) \). The band insulator is a map from the Brillouin zone \( T^d \) to \( Gr(n, m+n) \), which is related to the torus homotopy group \( \tau_d[Gr(n, m+n)] \) [7]. Since classes of mappings \( T^d \rightarrow Gr(n, m+n) \) are induced by classes of mappings \( S^d \rightarrow Gr(n, m+n) \), we shall focus on the latter.

In general \( \pi_3[Gr(n, m+n)] = 0 \), 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 \( C' \), this system always has an even number of bands, and its Hamiltonian belongs to the manifold \( M = Sp(2N)/U(N) \), and because \( \pi_3[Sp(2N)/U(N)] = \mathbb{Z}_2 \) for \( N > 1 \), the Hopf insulator has \( \mathbb{Z}_2 \) classification with symmetry \( C' \).

For a 2N-band system, the symmetry \( C' \) acts on fermion operators as \( C' f_i C'^{-1} = J f_i^J \). \( J \) 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 \( C' \) is a generalized particle-hole transformation, and it can be viewed as the product between a particle-hole transformation \( C \) (with \( C^2 = -1 \)) and the spatial inversion \( I \). The symmetry \( C' \) implies that for all \( \mathbf{k} \), the Hamiltonian \( H(\mathbf{k}) \) must satisfy

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

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

\[
H(\mathbf{k}) = \operatorname{diag}(\lambda_1(\mathbf{k}), -\lambda_1(\mathbf{k}), \lambda_2(\mathbf{k}), -\lambda_2(\mathbf{k}), \ldots, \lambda_N(\mathbf{k}), -\lambda_N(\mathbf{k})). \tag{8}
\]

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

\[
H(\mathbf{k}) = U(\mathbf{k}) I_{N,N} U^T(\mathbf{k}), \tag{9}
\]

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

\[
\pi_3[\text{Sp}(2N)/\text{U}(N)] = \begin{cases} 
Z & N = 1 \\
Z_2 & N \geq 2
\end{cases} \quad (11a)
\]

\[
\pi_4[\text{Sp}(2N)/\text{U}(N)] = Z_2 \quad (11b)
\]

The conclusion that the classification for the multi-band system with the \( C' \) symmetry is no larger than \( Z_2 \) can be understood as follows. Let us take \( N = 2 \). The nontrivial mapping from \( S^3 \) to \( \text{Sp}(4)/\text{U}(2) \) is induced by the mapping from \( S^3 \) to \( \text{Sp}(4) \), characterized by the winding number \( n_w = \frac{1}{2\pi^2} \int d^3k (U_{-1}^{-1}dU)^3 \), where \( U \in \text{Sp}(4) \). When \( n_w = 2 \), the induced Hamiltonian \( H(k) = U(k)I_{N,N}U(k) \) can be continuously deformed into two copies of two-band Hopf insulators each with the Hamiltonian Eq. (1), whose three-component vector \( \vec{n}(k)_1 = -\vec{n}(k)_2 \) (one can check that \( \vec{n}(k) \) and \( -\vec{n}(k) \) give the same Hopf number). Then it is obvious that this state should not have any edge state at the \( (0,0,1) \) boundary because each \( (k_r, k_z) \) half-plane for a fixed \( \theta \) now has zero Skyrminon number.

The classification for \( C' \) can be understood in another way. Under ordinary \( C \) transformation, the position variables are invariant, but all of the momenta variables pick up a sign. However, under the \( C' \) 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 \( C' \) with \( C \) as long as we reverse the roles of the position and momenta variables. Therefore, following Ref. [8] the classification of a \( d \)-dimensional TI with \( C' \) is the same as the classification of a \( \delta = 0 - d \equiv 8 - d(\text{mod} 8) \)-dimensional TI with \( C \), which is simply Class C. As expected, the classifications match for all \( d \).

We note that because the general multi-band model of the Hopf insulator requires the \( C' \) symmetry which involves spatial inversion, the boundary of the system necessarily breaks \( C' \) 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/superconductors with the ordinary inversion symmetry [9][11].

This heuristic picture of the Hopf insulator in Fig. 1 points the 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). A 3\( d \) Weyl semimetal [12] 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\(_2\) [13], 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 4\( d \) model. A 4\( d \) band structure is not just for pure theoretical interest, we can also view the fourth momentum as the time coordinate, and thus the entire band structure as a time-dependent 3\( d \) Hamiltonian. In 4\( d \), the set of maps \( S^4 \rightarrow Gr(n,m+n) \) is classified by \( \pi_4[\text{Gr}(n,m+n)] \). We will start with the minimal model \( m = n = 1 \). In this case, the band insulator is a map \( S^4 \rightarrow S^2 \), which has homotopy group \( \pi_4[S^2] = Z_2 \).

We need to construct a nontrivial map \( F: T^4 \rightarrow S^2 \). Heuristically this mapping can be viewed as the following: in the 4\( d \) 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 4\( d \) Hopf insulator constructed with the three component vector \( \vec{n} \) and Pauli matrices, can be heuristically viewed as “Chern-insulator \( \times T^2 \)”. Consequently, the 3\( d \) 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. [14]. 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 [15][16]. Pictorially,

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

where \( \Sigma f \) [17] is the reduced suspension of the Hopf map \( f \), defined as

\[
\Sigma f : (k,t) \mapsto (N_1, N_2, N_3, N_4),
\]

FIG. 3: The boundary zero energy states of the 4\( d \) minimal two-band model for Hopf insulator with \( m = 2 \) in Eq. (13) plotted in the 3\( d \) boundary Brillouin zone. Because this model can be heuristically viewed as “Chern-insulator \( \times T^2 \)”, its boundary has a torus of zero energy states.
where $\vec{N}$ is a four component vector with nonzero norm:

\[
N_1 = \sin(t/2)(\sin k_x \sin k_z + \sin k_y (m - \cos k_x - \cos k_y - \cos k_z)), \\
N_2 = \sin(t/2)(\sin k_x (m - \cos k_x - \cos k_y - \cos k_z) - \sin k_y \sin k_z), \\
N_3 = \cos t(\sin^2 k_x + \sin^2 k_y) + \sin^2 k_z + (m - \cos k_x - \cos k_y - \cos k_z)^2, \\
N_4 = \sin t((m - \cos k_x - \cos k_y - \cos k_z)^2 + \sin^2 k_z).
\]

(13)

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

\[
n_1(k, t, m) = 2(N_1N_3 + N_2N_4) \\
n_2(k, t, m) = 2(N_1N_4 - N_2N_3) \\
n_3(k, t, m) = N_1^2 + N_2^2 - N_3^2 - N_4^2.
\]

(14)

Finally, we define the Hamiltonian $H(k, t, m)$ (up to normalization) as

\[
H(k, t, m) = \vec{n}(k, t, m) \cdot \vec{\sigma}.
\]

(15)

The variable $t$ in this 4$d$ model can be viewed as time. This means we can consider our system as an adiabatic time-dependent band insulator, with a period of $2\pi$. In Fig. 3 we plot the zero energy states computed numerically at the boundary Brillouin zone of the minimal two-band model of the 4$d$ 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 multi-band system, and impose the $C'$ symmetry. With the $C'$ symmetry, there is still an even number of bands, and just like the 3$d$ story discussed before, since $\pi_4(\text{Sp}(N)/U(N)) = Z_2$ for all $N$, there is only one class of nontrivial Hopf insulator with the $C'$ symmetry.

In 4$d$ there is a well-known integer quantum Hall state without assuming any symmetry other than the charge conservation [18], but unlike the 2$d$ Chern-insulator, the 4$d$ integer quantum Hall state necessarily breaks the $C'$, because its response to the external electromagnetic field $j'_\mu \sim \epsilon_{\mu\nu\rho\tau} F_{\nu\rho} F_{\tau\sigma}$ breaks $C'$, where $j'_\mu$ is the charge current.

In summary, we found a class of 3$d$ and 4$d$ topological insulators whose topological nature is characterized by the Hopf map and its generalizations. We identified a $C'$ symmetry which gives these states a $Z_2$ 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 $C'$ symmetry becomes a special inversion symmetry $T'$ 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 $T'$ symmetry.

We gratefully acknowledge support from the Simons Center for Geometry and Physics, Stony Brook University, where some of the research for this paper was performed during the 2016 Simons Summer Workshop. The authors are supported by the David and Lucile Packard Foundation and NSF Grant No. DMR-1151208. The authors thank Sergio Cecotti, Dan Freed, Mike Hopkins, Joel E. Moore, and Ashvin Vishwanath for very helpful discussions. The first two authors of this work contributed equally.