Systematic construction of tight-binding Hamiltonians for topological insulators and superconductors

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A remarkable discovery in recent years is that there exist various kinds of topological insulators and superconductors characterized by a periodic table according to the system symmetry and dimensionality. To physically realize these peculiar phases and study their properties, a critical step is to construct experimentally relevant Hamiltonians that support these topological phases. We propose a general and systematic method based on the quaternion algebra to construct the tight-binding Hamiltonians for all the three-dimensional topological phases in the periodic table characterized by arbitrary integer topological invariants, which include the spin-singlet and the spin-triplet topological superconductors, the Hopf, and the chiral topological insulators as particular examples. For each class, we calculate the corresponding topological invariants through both geometric analysis and numerical simulation.

Topological insulators (TIs) and superconductors (TSCs) are symmetry-protected topological phases of noninteracting fermions described by quadratic Hamiltonians [1], which have robust gapless boundary modes protected by the system symmetry [2]. These protected boundary modes have exotic properties and in some cases are characterized as anyons with fractional statistics [3], which could be used for the realization of topological quantum computation [4]. Notable examples of TIs include the integer quantum Hall states [5] and the recently discovered two-dimensional (2D) quantum spin Hall states [6], and the three-dimensional (3D) $\mathbb{Z}_2$ TIs [7]. Examples of TSCs include the 2D $p + ip$ superconductors of spinless fermions [8] and the Helium superfluid B phase [9,10].

It turns out that the above TI/TSC examples are just a part of a larger scheme: they sit inside a periodic table for TIs/TSCs developed according to the symmetry and dimensionality of the system [9–11]. The periodic table predicts the possible existence of a number of new topological phases, and it is of great interest to search for these new phases in nature. However, the periodic table does not tell where to look for or how to realize these phases. To physically realize these exotic phases and study their properties, it is of critical importance to construct tight-binding Hamiltonians so that they could be realized in real quantum materials such as optical lattice systems [12]. So far, some clever example Hamiltonians have been found for a few new topological phases [11,13–15], typically with the topological invariant $\Gamma = \pm 1$, but we lack a systematic method to construct tight-binding Hamiltonians for generic topological phases with arbitrary integer topological invariants.

In this paper, we propose a general and systematic method to construct tight-binding Hamiltonians for new topological phases based on the use of quaternion algebra. By this method, we construct the tight-binding Hamiltonians for all the 3D topological phases in the periodic table with arbitrary integer topological invariants, which include the spin-singlet and the spin-triplet TSCs, the chiral and the Hopf TIs as prototypical examples. For each class, the topological invariant is explicitly calculated for the constructed Hamiltonian, using both geometric analysis and numerical simulation, which confirm that

we indeed realize all the topologically distinct phases in the corresponding class characterized by a topological invariant of arbitrary integer values. The construction method proposed here should also work for the 2D and 1D cases, and we believe its direct generalization to Clifford algebra should provide a powerful tool to construct tight-binding Hamiltonians for all the integer topological phases in the periodic table.

Before showing the method, let us first briefly introduce the quaternion algebra $\mathbb{H}$, which is a generalization of the familiar complex algebra, with the imaginary basis vectors extended from one ($\boldsymbol{i}$) to three ($\boldsymbol{i},\boldsymbol{j},\boldsymbol{k}$). The basis vectors ($\boldsymbol{i},\boldsymbol{j},\boldsymbol{k}$) multiply according to the following noncommutative product table [16]:

$$
\begin{aligned}
\boldsymbol{i}^2 = \boldsymbol{j}^2 = \boldsymbol{k}^2 = -1, \quad \boldsymbol{ij} = -\boldsymbol{ji} = \boldsymbol{k}, \\
\boldsymbol{jk} = -\boldsymbol{kj} = \boldsymbol{i}, \quad \boldsymbol{ki} = -\boldsymbol{ik} = \boldsymbol{j}.
\end{aligned}
\tag{1}
$$

Any element of $\mathbb{H}$ can be expanded as $q = q_0 + q_1 \boldsymbol{i} + q_2 \boldsymbol{j} + q_3 \boldsymbol{k}$, where q_i ($i = 0,1,2,3$) are real numbers. Quaternion has been used recently as a tool to analyze the 3D Landau levels [17,18].

For our purpose, it is more convenient to write q in the polarlike coordinate with $q = \rho(\cos\theta + \hat{\mathbf{a}}\sin\theta)$, where $\rho \equiv |q| = \sqrt{q_0^2 + q_1^2 + q_2^2 + q_3^2}$ is the norm of q, θ is the angle, and $\hat{\mathbf{a}} = \hat{a}_1 \boldsymbol{i} + \hat{a}_2 \boldsymbol{j} + \hat{a}_3 \boldsymbol{k}$ with $\hat{a}_1^2 + \hat{a}_2^2 + \hat{a}_3^2 = 1$ is a unity vector denoting the direction in the imaginary space. From the definition, we immediately get

$$
q^n = \rho^n (\cos n\theta + \hat{\mathbf{a}}\sin n\theta).
\tag{2}
$$

To construct tight-binding lattice Hamiltonians for the TIs or TSCs, we typically work in the momentum space. The Hamiltonian coefficients are taken as components q_i of a quaternion q, which in general depend on the momentum through the notation $q_i(\mathbf{k})$. In a d-dimensional ($d = 1,2,3$) space, the momentum $\mathbf{k}$ takes values from the Brillouin zone (BZ) characterized by a d-dimensional torus $\mathbb{T}^d$. The norm $|q|$ of the quaternion q characterizes the energy scale (energy gap) of the Hamiltonian, which can be taken as 1 (the energy unit) without loss of generality, and the topological space of q is thus characterized by the sphere $\mathbb{S}^d$. The Hamiltonian with $q_i(\mathbf{k})$ as

the coefficients can be considered as a map from the space $\mathbb{T}^d$ to $\mathbb{S}^d$. If this map is topologically nontrivial characterized by a topological invariant (usually taken as the winding number or Chern number) $\Gamma = 1$, geometrically (in the sense of homotopy) it means that the space $\mathbb{T}^d$ wraps around $\mathbb{S}^d$ one time through the map. Now consider a Hamiltonian where the coefficients are taken as the components of $q^n(\mathbf{k})$. From the geometric representation of q^n in the polar coordinate in Eq. (2), if the space $\mathbb{T}^d$ wraps around $\mathbb{S}^d$ one time through the map $\mathbf{k} \rightarrow q(\mathbf{k})$ with $\Gamma = 1$, it will wrap $\mathbb{S}^d$ n times through the map $\mathbf{k} \rightarrow q^n(\mathbf{k})$ with $\Gamma = n$. So, by this quaternion-power mapping, we can construct Hamiltonians for topologically distinct new phases with arbitrary integer topological invariants. This serves as our physical intuition to construct tight-binding Hamiltonians for new topological phases. In the following, we apply this method to construction of the Hamiltonians for all the 3D topological phases in the periodic table characterized by the integer group $\mathbb{Z}$, which include the spin-singlet and the spin-triplet TSCs, the chiral and the Hopf TIs.

Spin-singlet TSC (class CI). The topological phases in the periodic table are classified by three generic symmetries, the time reversal, the particle-hole exchange (charge conjugation), and the chiral symmetry, denoted respectively by T, C, S with $S \equiv TC$. These three symmetries can be used to classify the system even when weak disorder breaks the lattice translational symmetry. The symmetries T and C are represented by antiunitary operators, and T^2, C^2 can take values either $+1$ or -1 depending on the effective spin of the system.

Spin-singlet TSC is described by a Bogoliubov–de-Gennes (BdG) type of mean-field Hamiltonian and belongs to the symmetry class CI in the periodic table, which means the BdG Hamiltonian has both T and C symmetries with $T^2 = 1$ and $C^2 = -1$. The topological phase is characterized by a topological invariant Γ_{CI}, which takes values from $2\mathbb{Z}$ (even integers). Reference [19] has proposed a Hamiltonian in a diamond lattice, which realizes a special instance of the CI TSC with $\Gamma_{\text{CI}} = \pm 2$. Here, we construct tight-binding Hamiltonians that can realize all the topologically distinct phases for the CI TSC with arbitrary even integer Γ_{CI} in a simple cubic lattice. The simplified lattice geometry could be important for an experimental implementation.

To construct the BdG Hamiltonian in the momentum space, first we define a quaternion q with the following dependence on the momentum $\mathbf{k}$

$$q = t \cos k_x - \boldsymbol{i}(\sin k_x + \sin k_y + \sin k_z)$$
$$+ \boldsymbol{j} \cos k_y + \boldsymbol{k} \cos k_z, \tag{3}$$

where t is a dimensionless parameter. A family of the BdG Hamiltonians can be constructed on the 3D cubic lattice with the form $H_{\text{CI}} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} \mathcal{H}_{\text{CI}}(\mathbf{k}) \Psi_{\mathbf{k}}$ in the momentum space, where $\Psi_{\mathbf{k}} = (a_{\mathbf{k}\uparrow}, b_{\mathbf{k}\uparrow}, a_{-\mathbf{k}\downarrow}^{\dagger}, b_{-\mathbf{k}\downarrow}^{\dagger})^T$ denotes the fermionic mode operators with spin $\uparrow, \downarrow$ and momentum $\mathbf{k}$. The 4×4 Hamiltonian matrix reads

$$\mathcal{H}_{\text{CI}}(\mathbf{k}) = \begin{pmatrix} \mathbf{m} \cdot \boldsymbol{\sigma} & (q^n)_3 \mathbf{I}_2 \\ (q^n)_3 \mathbf{I}_2 & -\mathbf{m} \cdot \boldsymbol{\sigma} \end{pmatrix}, \tag{4}$$

where $\mathbf{m} = [(q^n)_0, (q^n)_1, (q^n)_2]$ with $(q^n)_i$ denoting the ith components of the quaternion q^n, $\mathbf{I}_2$ is the 2×2 identity

matrix, and $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ are the Pauli matrices. Expressed in the real space, the Hamiltonian H_{CI} contains spin-singlet d-wave pairing described by the quaternion component $(q^n)_3$, and has local hopping and pairing terms up to the nth neighboring sites. One can check that $\mathcal{H}_{\text{CI}}(\mathbf{k})$ indeed has both T and C symmetries (and thus also the chiral symmetry $S = TC$) with $T^2 = 1$ and $C^2 = -1$ (see the Appendix for an explicit check).

Now we show that the Hamiltonian H_{CI} has topologically distinct phases depending on the parameters n and t. For this purpose, we need to calculate the topological invariant Γ_{CI} for H_{CI}. Direct diagonalization of the Hamiltonian H_{CI} leads to the energy spectrum $E_{\pm}(\mathbf{k}) = \pm|q^n| = \pm\rho^n = \pm[t^2 \cos^2 k_x + \cos^2 k_y + \cos^2 k_z + (\sin k_x + \sin k_y + \sin k_z)^2]^{n/2}$. It is always gapped if $t \neq 0$ and has a twofold degeneracy for each $\mathbf{k}$. To calculate the topological index Γ_{CI}, we first flatten the bands of H_{CI} (which is a continuous transformation that does not change its topological property) by introducing the Q matrix,

$$Q(\mathbf{k}) = 1 - 2P(\mathbf{k}), \quad P(\mathbf{k}) = \sum_f |u_f(\mathbf{k})\rangle\langle u_f(\mathbf{k})|, \tag{5}$$

where $P(\mathbf{k})$ is the projector onto the filled Bloch bands [with energy $E_-(\mathbf{k})$ and wave vectors $|u_f(\mathbf{k})\rangle$ from the diagonalization of $\mathcal{H}_{\text{CI}}$]. With the chiral symmetry, the Q matrix can be brought into the block off-diagonal form $Q(\mathbf{k}) = \begin{pmatrix} 0 & b(\mathbf{k}) \\ b^{\dagger}(\mathbf{k}) & 0 \end{pmatrix}$ by a unitary transformation, with

$$b(\mathbf{k}) = - \begin{pmatrix} (q^n)_3 - i(q^n)_2 & -i(q^n)_0 - (q^n)_1 \\ -i(q^n)_0 + (q^n)_1 & (q^n)_3 + i(q^n)_2 \end{pmatrix} \Bigg/ E_+(\mathbf{k}) \tag{6}$$

for the Hamiltonian H_{CI}. With the matrix $b(\mathbf{k})$, the topological index Γ_{CI} is defined by the following winding number [10]:

$$\Gamma_{\text{CI}} = \frac{1}{24\pi^2} \int_{\text{BZ}} d\mathbf{k} \, \epsilon^{\mu\rho\lambda} \text{Tr}[(b^{-1}\partial_{\mu}b)(b^{-1}\partial_{\rho}b)(b^{-1}\partial_{\lambda}b)], \tag{7}$$

where $\epsilon^{\mu\rho\lambda}$ is the antisymmetric Levi-Civita symbol and $\partial_{\mu}b \equiv \partial_{k_{\mu}}b(\mathbf{k})$. When $n = 1$, the integral in Γ_{CI} can be calculated analytically and we find $\Gamma_{\text{CI}}(n = 1) = 2\text{sign}(t) = \pm 2$. In general cases, due to the geometric interpretation of the map q^n, we immediately get

$$\Gamma_{\text{CI}}[\mathcal{H}_{\text{CI}}] = 2n\text{sign}(t) = \pm 2n. \tag{8}$$

This result is confirmed through direct numerical calculations. We integrate Eq. (7) numerically through discretization of the Brillouin zone. The numerical results for different n are shown in Table I. As one varies n, it is evident from Eq. (8) that we can realize all the spin-singlet TSC phases in the CI class through our constructed Hamiltonian H_{CI} with the topological index Γ_{CI} taking arbitrary even integers.

Spin-triplet TSC (class DIII). Spin triplet TSCs are described by the BdG Hamiltonians that have both T and C symmetries with $T^2 = -1$ and $C^2 = 1$. It belongs to the symmetry class DIII in the periodic table. The ^{3}He superfluid B phase is a well known example in this class [9,10], but it is not described by a simple lattice model. Tight-binding lattice Hamiltonians have been constructed for the DIII-class spin triplet TSCs with the topological index $\Gamma_{\text{DIII}} = \pm 1$ [20–22].

TABLE I. Numerical results of the corresponding topological invariants for the constructed Hamiltonians in different symmetry classes. The symmetry property of each class is also indicated. The presence of time-reversal symmetry T, particle-hole symmetry C, and chiral symmetry S is denoted by ± 1, with ± 1 specifying the values of T^2 and C^2. The absence of these symmetries is denoted by 0. The parameters for the corresponding Hamiltonians are chosen as $(t,h) = (1,2)$. The number of grid points is $N_{grid} = 320$ for all the cases. The integer numbers in the square brackets are theoretical values for the corresponding topological invariants.

AZ class	Symmetry			Numerical results for different n				
	T	C	S	1	2	3	4	5
AIII	0	0	1	1.000 [1]	1.999 [2]	2.997 [3]	3.993 [4]	4.986 [5]
CI	1	−1	1	1.999 [2]	3.998 [4]	5.992 [6]	7.984 [8]	9.972 [10]
DIII	−1	1	1	1.000 [1]	1.999 [2]	2.997 [3]	3.993 [4]	4.986 [5]
A (HIs)	0	0	0	0.999 [1]	1.994 [2]	2.979 [3]	3.951 [4]	4.910 [5]

Here, we use the quaternion method to construct tight-binding Hamiltonians for the DIII-class TSCs with arbitrary integer topological indices Γ_{DIII} in a simple cubic lattice.

To construct the Hamiltonian, we define a quaternion $q(\mathbf{k})$ with the following dependence on $\mathbf{k}$

$$q = h + \cos k_x + \cos k_y + \cos k_z + \boldsymbol{i} t \sin k_x$$
$$+ \boldsymbol{j} \sin k_y + \boldsymbol{k} \sin k_z \qquad (9)$$

with t, h being dimensionless parameters. We will use this form of $q(\mathbf{k})$ for all our following examples. We construct a four-band BdG Hamiltonian with the form $H_{DIII} = \sum_{\mathbf{k}} \Phi_{\mathbf{k}}^{\dagger} \mathcal{H}_{DIII}(\mathbf{k}) \Phi_{\mathbf{k}}$, with the fermionic mode operators $\Phi_{\mathbf{k}} = (a_{\mathbf{k}\uparrow}, a_{\mathbf{k}\downarrow}, a_{-\mathbf{k}\uparrow}^{\dagger}, a_{-\mathbf{k}\downarrow}^{\dagger})^T$ and the 4×4 Hamiltonian matrix

$$\mathcal{H}_{DIII}(\mathbf{k}) = \mathbf{u} \cdot \boldsymbol{\Gamma}, \qquad (10)$$

where $\mathbf{u} = [(q^n)_1, (q^n)_2, (q^n)_3, (q^n)_0]$, $\boldsymbol{\Gamma} = (\gamma^0\gamma^1, \gamma^0\gamma^2, \gamma^0\gamma^3, -i\gamma^0\gamma^5)$, and γ^i denote the standard Dirac matrices with the explicit expressions given in the Appendix. This Hamiltonian has spin-triplet pairing with the energy spectrum $E_{\pm}(\mathbf{k}) = \pm|\mathbf{u}(\mathbf{k})| = \pm|q(\mathbf{k})|^n$, which is fully gapped when $|h| \neq 1, 3$ and $t \neq 0$.

The DIII class TSC has the chiral symmetry, so its Q matrix for the Hamiltonian can be brought into the block off-diagonal form (see Appendix) and the topological index Γ_{DIII} is also characterized by the winding number in Eq. (7). We find

$$\Gamma_{DIII}[\mathcal{H}_{DIII}] = \begin{cases} -2n\,\text{sign}(t) & |h| < 1 \\ n\,\text{sign}(t) & 1 < |h| < 3 \\ 0 & |h| > 3 \end{cases}. \qquad (11)$$

It is evident that the topological index Γ_{DIII} can take arbitrary integer values for our constructed Hamiltonian depending on the parameters n, t, h. In the particular case with $n = t = 1$, the Hamiltonian reduces to the model Hamiltonian introduced in Refs. [10,11], which has $\Gamma_{DIII} = 1$ or -2.

Chiral TI (class AIII). Chiral TIs do not have time-reversal or particle-hole symmetry (thus $T = C = 0$), but they possess chiral symmetry with $S = 1$ and belongs to the symmetry class AIII in the periodic table. Tight-binding Hamiltonians have been constructed for the chiral TIs with the topological index $\Gamma_{AIII} = \pm 1$ [23]. Here, we use the quaternion method to construct Hamiltonians with arbitrary integer Γ_{AIII}. We consider a three-band Hamiltonian with the following form $H_{AIII} = \sum_{\mathbf{k}} \xi_{\mathbf{k}}^{\dagger} \mathcal{H}_{AIII}(\mathbf{k}) \xi_{\mathbf{k}}$, where the fermionic mode operators

$\xi_{\mathbf{k}} = (a_{\mathbf{k}}, b_{\mathbf{k}}, c_{\mathbf{k}})^T$ and the 3×3 Hamiltonian matrix

$$\mathcal{H}_{AIII}(\mathbf{k}) = \mathbf{u} \cdot \mathcal{G}. \qquad (12)$$

In $\mathcal{H}_{AIII}$, $\mathbf{u}$ denotes the same quaternion coefficients as defined below Eq. (10) and $\mathcal{G} = (\lambda_4, \lambda_5, \lambda_6, \lambda_7)$ are the four Gell-Mann matrices with the explicit form given in the Appendix. The Hamiltonian H_{AIII} is gapped when $|h| \neq 1, 3$ and $t \neq 0$ and has a perfectly flat middle band with a macroscopic number of zero-energy modes due to the chiral symmetry [23]. A topological invariant classifying this family of Hamiltonians can be defined as [23]

$$\Gamma_{AIII} = -\frac{1}{12\pi^2} \int_{BZ} d\mathbf{k}\, \epsilon^{\alpha\beta\gamma\rho} \epsilon^{\mu\nu\tau} \frac{1}{|\mathbf{u}|^4} \mathbf{u}_{\alpha} \partial_{\mu}\mathbf{u}_{\beta} \partial_{\nu}\mathbf{u}_{\gamma} \partial_{\tau}\mathbf{u}_{\rho}. \qquad (13)$$

We have calculated this invariant and found that

$$\Gamma_{AIII}[\mathcal{H}_{AIII}] = n\,\text{sign}(t) = \pm n, \quad (1 < |h| < 3) \qquad (14)$$

for our constructed H_{AIII}. This analytic result is confirmed with direct numerical calculations as shown in Table I. In the particular case with $n = 1$, the Hamiltonian H_{AIII} reduces to the model Hamiltonian constructed in Ref. [23]. Through the quaternion power, we extend the model Hamiltonian and realize the chiral TIs with the topological index taking arbitrary integer values.

Hopf insulators (class A). The Hamiltonians in class A do not have any symmetry (T, C, or S) except the particle number conservation. Generically, this class of Hamiltonians have no topologically nontrivial phase in 3D, but there is a peculiar exception, called the Hopf insulator, which occurs when the Hamiltonian has just two bands due to the existence of the topologically nontrivial Hopf map from $\mathbb{S}^3$ to $\mathbb{S}^2$ [15,24]. To understand why Hopf insulators exist, note that the space of all 3D band Hamiltonians with m filled and n empty bands is topologically equivalent to the Grassmannian manifold $\mathbb{G}_{m,n+m}$ and can be classified by the homotopy group of this Grassmannian [11]. Since $\pi_3(\mathbb{G}_{m,n+m}) = 0$ for all $(m,n) \neq (1,1)$, no nontrivial topological phase exists in general. However, when $m = n = 1$, $\mathbb{G}_{1,2}$ is topologically equivalent to two-sphere $\mathbb{S}^2$ and $\pi_3(\mathbb{G}_{m,n+m}) = \pi_3(\mathbb{S}^2) = \mathbb{Z}$. This explains why the Hopf insulators may exist in three dimensions. The Hopf insulators are characterized by the topological Hopf index Γ_H, which takes values from the integer set $\mathbb{Z}$. A model Hamiltonian has been constructed

for the Hopf insulator with $\Gamma_H = \pm 1$ in Ref. [15] based on the Hopf map [25]. This method was extended in Ref. [24] to construct Hamiltonians for general Hopf insulators with arbitrary integer Γ_H based on the generalized Hopf map encountered in mathematics but not in physics literature. Here, with the quaternion algebra, we use only the simple Hopf map but still can construct tight-binding Hamiltonians for the Hopf insulators with arbitrary integer Γ_H.

To construct the Hamiltonian, we define two complex variables $\eta = (\eta_\uparrow, \eta_\downarrow)^T$ from the quaternion $\eta_\uparrow = (q^n)_1 + i(q^n)_2$, $\eta_\downarrow = (q^n)_3 + i(q^n)_0$, where $q(\mathbf{k})$ is defined by Eq. (9). The Hopf map is defined as $\mathbf{v} = \eta^\dagger \boldsymbol{\sigma} \eta$, which is a quadratic map from $\mathbb{S}^3 \to \mathbb{S}^2$ up to normalization. The two-band Hamiltonians can then be constructed as $H_{\text{Hopf}} = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger \mathcal{H}_{\text{Hopf}}(\mathbf{k}) \psi_{\mathbf{k}}$ with $\psi_{\mathbf{k}} = (a_{\mathbf{k}\uparrow}, a_{\mathbf{k}\downarrow})^T$ and

$$\mathcal{H}_{\text{Hopf}}(\mathbf{k}) = \mathbf{v} \cdot \boldsymbol{\sigma}. \tag{15}$$

The Hopf insulators are characterized by the topological Hopf index, defined as

$$\Gamma_H[\mathcal{H}_{\text{Hopf}}] = -\int_{\text{BZ}} \mathbf{F} \cdot \mathbf{A} \, d^3\mathbf{k}, \tag{16}$$

where $\mathbf{F}$ is the Berry curvature with $F_\mu \equiv \frac{1}{8\pi} \epsilon_{\mu\nu\tau} \mathbf{v} \cdot (\partial_\nu \mathbf{v} \times \partial_\tau \mathbf{v})$ and $\mathbf{A}$ is the associated Berry connection, which satisfies $\nabla \times \mathbf{A} = \mathbf{F}$ [15,24]. From this definition and our geometric interpretation of q^n, we find

$$\Gamma_H[\mathcal{H}_{\text{Hopf}}] = n \, \text{sign}(t) = \pm n, \quad (1 < |h| < 3). \tag{17}$$

This analytical expression is also confirmed with direct numerical calculations. Some numerical results for the topological indices are listed in Table I for different classes of TIs and TSCs, which agree very well with our analytical expressions.

It is noteworthy to point out that although the geometric picture is intuitive, it is not a mathematically rigorous proof. We therefore have done substantial numerical calculations to support our conclusion and parts of our results are shown in Table I. All results are in line with the geometric argument and the topological invariants indeed have values proportional to the power n of the quaternions. Another subtlety to note is that we did not define the same quaternion for all four examples. This has its root in the parity restriction for each component of the quaternion. In the construction of $\mathcal{H}_{\text{CI}}^{(n)}(\mathbf{k})$, the symmetries require three components of the quaternion q to have even parity under the exchange $\mathbf{k} \to -\mathbf{k}$ and the remaining component odd parity. However, for $\mathcal{H}_{\text{DIII}}^{(n)}(\mathbf{k})$, three components should be odd and the other even. As a result, different quaternions are chosen for these two classes. We wish to underline the important fact that q^n preserves the parity property of q defined above. This crucial property of quaternion algebra enables us to write down a unified expression for Hamiltonians of each symmetry class with arbitrary integer topological index.

Before ending the paper, we briefly remark that the quaternion tool proposed here can be extended straightforwardly to the 1D and 2D cases although our focus in this paper is on the 3D topological phases. We can set one (two) of the quaternion components to zero for the 2D (1D) case and observe that the map $q \longrightarrow q^n$ always preserves the subspace of $\mathbb{H}$ spanned by $\{1, \boldsymbol{i}, \boldsymbol{j}\}$ ($\{1, \boldsymbol{i}\}$). With the power mapping

q^n, which preserves the symmetry of the Hamiltonian, starting from one particular example of topological Hamiltonians with the topological index $\Gamma = \pm 1$, we can always construct a family of Hamiltonians that realize all the topological phases with arbitrary integer Γ. Another interesting topic is to study the application of our quaternion toolkit in interacting systems and how interaction will affect our constructed Hamiltonians. In the small interaction limit, our constructions should not be affected because of the finite energy gap in the constructed Hamiltonians.

In summary, we have proposed a powerful tool based on the quaternion algebra to systematically construct tight-binding Hamiltonians for all the topological phases in the periodic table that are characterized by arbitrary integer topological indices. The constructed Hamiltonians make the basis for further studies of properties of these topological phases and phase transitions and provide an important step for future experimental realization.

APPENDIX: SYMMETRY CHECK AND THE CALCULATION OF TOPOLOGICAL INDICES

In this Appendix, we explicitly check the symmetries for our constructed Hamiltonians. We also give some details for the description of these Hamiltonians and the calculation of their corresponding topological indices.

We first specify the definition of time-reversal (T), particle-hole (charge conjugation C), and chiral ($S = TC$) symmetries in the momentum ($\mathbf{k}$) space. A Hamiltonian is represented by a finite matrix $\mathcal{H}(\mathbf{k})$ in the $\mathbf{k}$ space (kernel of the Hamiltonian). It has the time-reversal symmetry if there exists a unitary matrix T_m such that

$$T_m \mathcal{H}^*(\mathbf{k}) T_m^{-1} = \mathcal{H}(-\mathbf{k}). \tag{A1}$$

Similarly, $\mathcal{H}(\mathbf{k})$ has the particle-hole symmetry if there is a unitary matrix C_m such that

$$C_m \mathcal{H}^*(\mathbf{k}) C_m^{-1} = -\mathcal{H}(-\mathbf{k}). \tag{A2}$$

The antiunitary nature of the time-reversal and the particle-hole symmetries is manifested in the complex conjugate $\mathcal{H}^*(\mathbf{k})$ in Eqs. (1) and (2). Finally, as $S = TC$, the chiral symmetry is unitary and represented by ($S_m = T_m C_m^*$)

$$S_m \mathcal{H}(\mathbf{k}) S_m^{-1} = -\mathcal{H}(\mathbf{k}). \tag{A3}$$

Pertaining to the presence/absence of these symmetries, ten classes of single-particle Hamiltonians can be specified, which is intimately related to the classification of random matrices by Altland and Zirnbauer (AZ) [26].

1. Spin-singlet topological superconductor

We first prove that the Hamiltonian H_{CI} for the spin-singlet topological superconductors (TSCs) constructed in Eq. (4) of the main text has the CI-class symmetry with $T^2 = 1$ and $C^2 = -1$. Let us denote the parity of a function $f(\mathbf{k})$ by $P[f(\mathbf{k})]$, with $P = 1$ (-1) for an even (odd) parity under the exchange $\mathbf{k} \to -\mathbf{k}$. From the product table of the quaternion algebra, it is easy to check that with $P[(q)_1] = P[(\sin k_x + \sin k_y + \sin k_z)] = -1$ and $P[(q)_0] = P[(q)_2] = P[(q)_3] = 1$, we have $P[(q^n)_0] = P[(q^n)_2] = P[(q^n)_3] = 1$ and $P[(q^n)_1] = -1$ for any integer power n. The explicit expression of the Hamiltonian in Eq. (4) of the main text is

$$\mathcal{H}_{CI}(\mathbf{k}) = \begin{pmatrix} (q^n)_2 & (q^n)_0 - i(q^n)_1 & (q^n)_3 & 0 \\ (q^n)_0 + i(q^n)_1 & -(q^n)_2 & 0 & (q^n)_3 \\ (q^n)_3 & 0 & -(q^n)_2 & -(q^n)_0 + i(q^n)_1 \\ 0 & (q^n)_3 & -(q^n)_0 - i(q^n)_1 & (q^n)_2 \end{pmatrix}. \tag{A4}$$

From the parity of q^n, the time-reversal symmetry can be readily seen as

$$[\mathcal{H}_{CI}(\mathbf{k})]^* = \mathcal{H}_{CI}(-\mathbf{k}), \tag{A5}$$

so $T_m = \mathbf{I}_4$, the 4×4 identity matrix. The particle-hole symmetry can be seen as

$$C_m[\mathcal{H}_{CI}(\mathbf{k})]^* C_m^{-1} = -\mathcal{H}_{CI}(-\mathbf{k}), \tag{A6}$$

with $C_m = \mathbf{I}_2 \otimes \sigma^y$, where $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ denote the Pauli matrices. Apparently, $T^2 = 1$ and $C^2 = -1$ (as $C_m C_m^* = -\mathbf{I}_4$), as it is the case for the CI-class symmetry.

To calculate the topological invariant, we note that the system also has the chiral symmetry $S = TC$ and the $Q(\mathbf{k})$ matrix (defined in the main text) can thus be brought into the block off-diagonal form by a unitary transformation [10,11]. At the half filling (therefore inside the energy gap) and with a convenient gauge, direct calculation leads to

$$Q(\mathbf{k}) = \begin{pmatrix} 0 & b(\mathbf{k}) \\ b^\dagger(\mathbf{k}) & 0 \end{pmatrix}, \quad b(\mathbf{k}) = -\begin{pmatrix} (q^n)_3 - i(q^n)_2 & -i(q^n)_0 - (q^n)_1 \\ -i(q^n)_0 + (q^n)_1 & (q^n)_3 + i(q^n)_2 \end{pmatrix} \Big/ E_+(\mathbf{k})$$

with $E_+(\mathbf{k}) = |q(\mathbf{k})|^n$, as mentioned in the main text.

2. Spin-triplet topological superconductor

The Dirac matrices (also known as the γ matrices) $\{\gamma^0, \gamma^1, \gamma^2, \gamma^3\}$ are a set of 4×4 matrices, defined as

$$\gamma^0 = \begin{pmatrix} \mathbf{I}_2 & \mathbf{0} \\ \mathbf{0} & -\mathbf{I}_2 \end{pmatrix}, \quad \gamma^1 = \begin{pmatrix} \mathbf{0} & \sigma^x \\ -\sigma^x & \mathbf{0} \end{pmatrix}, \quad \gamma^2 = \begin{pmatrix} \mathbf{0} & \sigma^y \\ -\sigma^y & \mathbf{0} \end{pmatrix}, \quad \gamma^3 = \begin{pmatrix} \mathbf{0} & \sigma^z \\ -\sigma^z & \mathbf{0} \end{pmatrix},$$

The fifth γ matrix is defined by $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \sigma^x \otimes \mathbf{I}_2$. Using the explicit form of these γ matrices, the Hamiltonian matrix $\mathcal{H}_{DIII}(\mathbf{k})$ can be written as

$$\mathcal{H}_{DIII}(\mathbf{k}) = \begin{pmatrix} 0 & 0 & -i(q^n)_0 + (q^n)_3 & (q^n)_1 - i(q^n)_2 \\ 0 & 0 & (q^n)_1 + i(q^n)_2 & -i(q^n)_0 - (q^n)_3 \\ i(q^n)_0 + (q^n)_3 & (q^n)_1 + i(q^n)_2 & 0 & 0 \\ (q^n)_1 - i(q^n)_2 & i(q^n)_0 - (q^n)_3 & 0 & 0 \end{pmatrix}. \tag{A7}$$

The $Q(\mathbf{k})$ matrix can thus be written as

$$Q(\mathbf{k}) = \begin{pmatrix} 0 & b(\mathbf{k}) \\ b^\dagger(\mathbf{k}) & 0 \end{pmatrix}, \quad b(\mathbf{k}) = -\begin{pmatrix} -i(q^n)_0 + (q^n)_3 & (q^n)_1 - i(q^n)_2 \\ (q^n)_1 + i(q^n)_2 & -i(q^n)_0 - (q^n)_3 \end{pmatrix} \Big/ E_+(\mathbf{k}),$$

with $E_+(\mathbf{k}) = |q(\mathbf{k})|^n$. Note that for the quaternion q defined in Eq. (9) of the main text, we have $P[(q)_1] = P[(q)_2] = P[(q)_3] = -P[(q)_0] = -1$ and thus $P[(q^n)_1] = P[(q^n)_2] = P[(q^n)_3] = -P[(q^n)_0] = -1$. With the parity properties, one can easily check that

$$(\sigma_x \otimes \sigma_y)[\mathcal{H}_{DIII}(\mathbf{k})]^*(\sigma_x \otimes \sigma_y) = \mathcal{H}_{DIII}(-\mathbf{k}), \tag{A8}$$

$$(\sigma_y \otimes \sigma_y)[\mathcal{H}_{DIII}(\mathbf{k})]^*(\sigma_y \otimes \sigma_y) = -\mathcal{H}_{DIII}(-\mathbf{k}). \tag{A9}$$

So the symmetry matrix $T_m = \sigma_x \otimes \sigma_y$ and $C_m = \sigma_y \otimes \sigma_y$ with $T^2 = -1$ and $C^2 = 1$ (as $T_m T_m^* = -\mathbf{I}_4$ and $C_m C_m^* = \mathbf{I}_4$), as it is the case for the DIII-class symmetry.

3. Chiral topological insulator

The four Gell-Mann matrices used in the text are defined as

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$

The Hamiltonian matrix $\mathcal{H}_{\text{AIII}}(\mathbf{k})$ for the chiral topological insulator has the following explicit form

$$\mathcal{H}_{\text{AIII}}(\mathbf{k}) = \begin{pmatrix} 0 & 0 & (q^n)_1 - i(q^n)_2 \\ 0 & 0 & (q^n)_3 - i(q^n)_0 \\ (q^n)_1 + i(q^n)_2 & (q^n)_3 + i(q^n)_0 & 0 \end{pmatrix}.$$

The Hamiltonian $\mathcal{H}_{\text{AIII}}(\mathbf{k})$ does not have time-reversal or particle-hole symmetry, but it has a chiral symmetry $S_m \mathcal{H}_{\text{AIII}}(\mathbf{k}) S_m^{-1} = -\mathcal{H}_{\text{AIII}}(\mathbf{k})$ with the unitary matrix

$$S_m = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{A10}$$

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