Green’s Function Approach to Interacting Higher-order Topological Insulators

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The Bloch wave functions have been playing a crucial role in the diagnosis of topological phases in non-interacting systems. However, the Bloch waves are no longer applicable in the presence of finite Coulomb interaction and alternative approaches are needed to identify the topological indices. In this paper, we focus on three-dimensional higher-order topological insulators protected by $C_4T$ symmetry and show that the topological index can be computed through eigenstates of inverse Green’s function at zero frequency. If there is an additional $S_4$ rotoinversion symmetry, the topological index $P_3$ can be determined by eigenvalues of $S_4$ at high symmetry momenta, similar to the Fu-Kane parity criterion. We verify this method using many-body exact diagonalization in higher-order topological insulators with interaction. We also discuss the realization of this higher-order topological phase in tetragonal lattice structure with $C_4T$-preserving magnetic order. Finally, we discuss the boundary conditions necessary for the hinge states to emerge and show that these hinge states exist even when the boundary is smooth and without a sharp hinge.

I. INTRODUCTION

Topological phases of matter are characterized by an exotic bulk-boundary correspondence that enforces the boundary to be gapless although the bulk has a finite energy gap. The first-order topological insulators in $d$-dimension have $(d-1)$-dimensional in-gap boundary states that are robust to perturbations as long as the bulk gap remains open and the symmetries are not broken by perturbations$^{1-7}$. The higher-order topological insulators have in-gap states at $(d-n)$-dimensional boundary$^{8-39}$, e.g., the second-order topological insulators in three-dimensional space have gapless hinge states. These non-trivial topological features are indicated by topological indices. For non-interacting systems, the Bloch wave functions have been playing an important role in the diagnosis of topological phases. From the Berry curvature for Chern insulators to the nested Wilson loop$^{30-40}$ for higher order topological insulators, all these quantities involve Bloch wave functions. The representation of Bloch wave functions under symmetry groups also enables a highly efficient approach to identify topological phases regardless of the microscopic details in materials$^{41-52}$.

The presence of Coulomb interaction poses several challenges in characterizing the topological properties of electronic systems. Firstly, some of the topological phases may not be stable under interaction, and interaction can modify the topological classification. For example, the topological classification of one-dimensional Majorana chain can be reduced from $Z$ to $Z_8$ by interaction$^{30}$. Secondly, topological indices in non-interacting electronic systems are usually defined in terms of Bloch wave functions, which can only capture information in the single-particle Hamiltonian and cannot describe correlation effects. Therefore, in the presence of interaction it is desirable to find an alternative approach that can take into account the many-body physics and characterize the topological properties of the interacting system$^{45-60}$.

The well-known Chern insulators and time-reversal protected $\mathbb{Z}_2$ topological insulators are examples of first-order topological insulators that are known to be robust under weak Coulomb interaction which does not close the band gap$^2$. Furthermore, Wang, Qi and Zhang$^{61-63}$ suggested when there is finite interaction in these systems, the role of Bloch wave functions can be played by the eigenstates of the inverse Green’s function at zero frequency such that the topological indices can be formulated through these eigenstates.

For higher-order topological phases, however, the fate of topological features under interaction becomes less clear. For example, Ref. 64 questioned the stability of the three-dimensional $C_4T$-protected second order topological insulator$^{10}$ under weak Coulomb interaction ($C_4$ is fourfold rotation and $T$ is time-reversal), which raised a debate on whether a weak Coulomb interaction is sufficient to destroy the higher-order topological insulators$^{54-66}$. Therefore, how to characterize higher-order topological phases in the presence of interaction still remains an open question.

In this paper, we study the topological properties and stability of higher-order topological insulators under interaction. We focus on the $C_4T$-protected three dimensional second order topological insulator with interaction and show that its topological index can be computed in a gauge-independent way through eigenstates of the inverse Green’s function at zero frequency, which is a generalization of the approach in Ref. 61 and 62. Furthermore, if there is an $S_4$ rotoinversion symmetry in addition to $C_4T$, the topological index $P_3$ in this interacting system can be determined by eigenvalues of $S_4$ at high symmetry momenta, similar to the Fu-Kane parity criterion$^9$. We demonstrate this method by computing the topological index of HOTIs with Coulomb interaction, where we obtain the Green’s function from exact diagonalization (ED). We also discuss the realization of this higher-order topological phase in insulators with $C_4T$-preserving magnetic order. Finally, we investigate the influence of Coulomb interaction and boundary termination on the hinge states. We show that the gapless hinge states as the features of higher-order topology remain robust under weak Coulomb interaction that does not close the surface gap, and the hinge states can emerge even when boundary is smooth and without a sharp hinge.
Consider the 3D chiral second-order topological insulator protected by \( C_4T \) symmetry proposed in Ref. 10. The higher-order topological feature is characterized by the chiral hinge states propagating in alternating directions at hinges parallel to the fourfold rotational axis, as shown in Fig. 1(a). In the non-interacting limit, a tight-binding model for this second-order topological insulator is given by

\[
H_0(k) = \left[ M + \sum_{i=x,y,z} t_i \cos(k_i a) \right] \tau_z \sigma_0 + \sum_{i=x,y,z} \Delta_i \sin(k_i a) \\
\times \tau_x \sigma_i + A_1 \sin(k_z a) \tau_y \sigma_0 + A_2 \tau_x \sigma_0 \\
+ \Delta_2 \left[ \cos(k_x a) - \cos(k_y a) \right] \tau_y \sigma_0.
\]  

(1)

Here \( \tau \) and \( \sigma \) refer to the orbital and spin spaces respectively. The fourfold rotation operator is \( C_4 = \tau_0 e^{i \pi \sigma_z} \) and time-reversal operator is \( T = -i \tau_0 \sigma_z K \), where \( K \) is complex conjugation. Without the \( \Delta_2 \) term, the system is a first-order \( Z_2 \) topological insulator with symmetries \( C_4 \) and \( T \). The \( \Delta_2 \) term breaks \( C_4 \) and \( T \) separately but preserves the product \( C_4T \), which opens a surface gap and drives the system into a second-order topological insulator protected by \( C_4T \) symmetry. The topological index for this system is the magneto-electric polarization

\[
\mathcal{P}_{\text{larization}} = \frac{\text{tr} \mathcal{S}}{8 \pi^2} \sum_{\tau_{1/2}} \int d^3k \epsilon^{ijk} \text{Tr} \left[ \partial_i \mathcal{A}_j(k) + \frac{2}{3} i \mathcal{A}_i(k) \mathcal{A}_j(k) \right] \mathcal{A}_k(k).
\]  

(3)

Here \( \mathcal{A}_j(k) \) is an \( N_x \times N_y \) matrix defined from the eigenstates of \( G^{-1}(0,k) \) with positive eigenvalues:

\[
\left[ \mathcal{A}_j(k) \right]_{mn} = -i \langle g_m(k) | \frac{\partial}{\partial k_i} | g_n(k) \rangle, \quad \lambda_m(k), \lambda_n(k) > 0.
\]  

(4)

Although Eq.(4) is similar to the non-Abelian Berry connection in the non-interacting systems, the physical meaning is very different, because Eq.(4) involves the eigenstates of inverse Green’s function at zero frequency rather than Bloch wave functions. Eq.(3) is well-defined for interacting systems, but the direct computation from Eq.(3) is not practical due to the requirement of a global smooth gauge in \( \mathcal{A}_j(k) \).

The symmetries in higher-order topological insulator can further simplify Eq.(3) so that a global smooth gauge is no longer needed. \( C_4T \) symmetry requires

\[
(C_4T)G^{-1}(i\omega, k)(C_4T)^{-1} = G^{-1}(-i\omega, C_4Tk),
\]  

(5)

where \( C_4Tk = (k_y, -k_x, -k_z) \). This implies \( C_4T|g_n(k)\rangle \) is an eigenstate of \( G^{-1}(0, C_4Tk) \) with the same energy. Therefore, the \( C_4T|g_n(k)\rangle \) can be expanded as \( C_4T|g_n(k)\rangle = \sum_m |g_m(C_4Tk)\rangle B(k)_{mn} \) and the sewing matrix \( B(k) \) is unitary:

\[
B(k)_{mn} = \langle g_m(C_4Tk) | C_4T | g_n(k) \rangle.
\]  

(6)

The similarity between Eqs.(3)-(6) and their Bloch counterpart in the non-interacting limit implies \( P_3 \) can be written as the wrapping number of sewing matrix \( B(k) \)\(^{10}\).

\[
2P_3 = -\frac{1}{24\pi^2} \int d^3k \epsilon^{ijk} \text{Tr} \left[ \left( B \partial_i B^i \right) \left( B \partial_j B^j \right) \left( B \partial_k B^k \right) \right].
\]  

(7)

Using the degree counting method in Ref. 67, Eq.(7) can be
reduced to a Pfaffian formula:
\[ 2P_3 = \frac{1}{2\pi i} \oint_{\partial \tau_{1/2}} dk \cdot \nabla \log \text{Pf}[M(k)], \tag{8} \]
\[ M(k)_{mn} = \langle g_m(k) | C_4 T + C_4^{-1} T | g_n(k) \rangle. \tag{9} \]

Here Pf denotes Pfaffian, which is only defined for antisymmetric matrices. The anti-symmetric property of matrix \( M \) is guaranteed by \((C_4 T)^4 = -1\), as shown in the appendix. \( \partial \tau_{1/2} \) is the boundary of the region \( \tau_{1/2} \) in Fig.1(b). Because the integral along \( ZA \) and \( Z' A' \) cancel each other by periodicity, the integral only involves \( ZZ' \) and \( AA' \). Importantly, to evaluate Eq.(8) one needs to make a gauge choice such that \( \det[B(k)] \) is smooth in \( \tau_{1/2} \).

Starting from the Pfaffian formula Eq.(8), a gauge-independent method can be developed to compute the topological index \( P_3 \), which only involves the inverse Green’s function at momenta inside \( \tau_{1/2} \). Define a gauge-invariant quantity \( \mathcal{R} \) on a straight line connecting \( k_a \) and \( k_b \) in momentum space:
\[ \mathcal{R}(k_a, k_b) = \frac{\text{Pf}[M(k_b)]}{\text{Pf}[M(k_a)]} \det[W(k_a, k_b)], \tag{10} \]
\[ W_{mn}(k_a, k_b) = \langle g_m(k_a) | \prod_{k_i \in k_a k_b} P_{k_i} | g_n(k_b) \rangle. \tag{11} \]

Here \( P_k = \sum_m |g_m(k)\rangle \langle g_m(k)| \) is the projection to the space spanned by eigenstates of inverse Green’s function with positive eigenvalues, and \( \overrightarrow{k_a k_b} \) denotes the straight line connecting \( k_a \) and \( k_b \). The arrow \( k_a \leftarrow k_b \) denotes the direction of path-ordered product which puts momentum points close to \( k_b \) to the right. The path-ordered product in \( W \) is similar to the Wilson loop but it is defined in interacting systems. Let \( G_0 \) be the vector connecting \( \Gamma \) and \( M \) points in the Brillouin zone. As shown in the appendix, \( \mathcal{R}(k_a, k_b) \) is invariant under gauge transformation \( |g_n(k)\rangle \rightarrow \sum_m |g_m(k)\rangle U_{mn}(k) \) and the Pfaffian formula in Eq.(8) can be computed by the following integral along the straight line connecting \( Z' \) and \( Z^{08} \):
\[ 2P_3 = \frac{1}{2\pi i} \int_{Z'} dk \cdot \nabla \log \mathcal{R}(k, k + G_0). \tag{12} \]

Eq.(12) can be understood as follows. It can be shown that \( \mathcal{R}(k_a, k_b) \) reduces to the ratio of the Pfaffian of \( M \) matrix between \( k_b \) and \( k_a \) under a suitable gauge choice. Then Eq.(12) measures the winding of the phase of Pfaffian along \( ZZ' \) and \( AA' \), which is equivalent to Eq.(8). A more rigorous proof is shown in the appendix. In practical computation, the path-ordered product in \( W \) can be evaluated at discrete momentum points similar to the computation of Wilson loop because the phase of \( W \) is insensitive to discretization of momentum points. Due to the gauge-invariance of \( \mathcal{R} \), the evaluation of Eq.(12) does not require a smooth gauge, and it can be computed in any gauge obtained directly from diagonalizing the inverse Green’s function. Therefore Eq.(12) provides an efficient gauge-independent method for computing topological index \( P_3 \) in interacting systems.

If the system has a fourfold rotoinversion symmetry \( S_4 = C_4 I \) in addition to \( C_4 T \) symmetry where \( I \) denotes space inversion operator, the eigenstates \( |g_n(k)\rangle \) of \( G^{-1}(0, k) \) at \( S_4 \)-invariant momentum \( k \) are also simultaneous eigenstates of \( S_4 \), leading to
\[ S_4 |g_n(k)\rangle = s_n |g_n(k)\rangle, \quad k \in K^4. \tag{13} \]

Here \( K^4 \) is the set of four high symmetry momenta that are invariant under \( S_4 \) in the 3D Brillouin zone, as shown in Fig.1(b). Following Ref. 67, in the presence of \( S_4 \) symmetry Eq.(8) can be simplified to the product of \((s_n + s_n^{-1})/\sqrt{2} = \pm 1 \) at high symmetry momenta:
\[ (-1)^{2P_3} = \prod_{k \in K^4} \prod_n \left| \frac{s_n(k) + s_n^{-1}(k)}{\sqrt{2}} \right| . \tag{14} \]

Here the product of \( n \) is over the eigenstates of \( G^{-1}(0, k) \) with positive eigenvalues, and only one state in each Kramers pair is taken in the product. Eq.(14) shows that in the presence of finite interaction, although Bloch wave functions can no longer be applied to compute topological index, an alternative route is provided by the eigenstates of inverse Green’s function at zero frequency such that topological indices can still be extracted from eigenvalues of symmetry operators.

### III. GREEN’S FUNCTION METHOD IN OTHER HIGHER-ORDER TOPOLOGICAL PHASES

The Green’s function method can also be applied to some other types of higher-order topological insulators with interaction. For example, the 3D helical HOTI proposed in Ref.10 is protected by time-reversal symmetry and a pair of perpendicular mirror symmetries \( M_{xy} \) and \( M_{x'y'} \). The hinge states appear at the mirror-invariant hinges when the corresponding mirror Chern number \( C_m \) is a nonzero even number. The two mirror symmetries constitutes a \( \mathbb{Z} \times \mathbb{Z} \) classification and the topological index is \( C_m/2 \). When there is finite interaction, the Bloch wave functions are not available to compute the mirror Chern number, but it can still be computed from the eigenstates of the inverse Green’s function obtained in Eq.(2). Because the inverse Green’s function still preserves mirror symmetry, one can select out the eigenstate \( |g(k)\rangle \) of inverse Green’s function that is simultaneous eigenstate of the mirror symmetry. Then the effective Berry connection is given by \( \mathcal{A}_f(k) = -i\langle g(k) | \partial_k | g(k) \rangle \) and the mirror Chern number can be computed by \( C_m = \int d^2k \partial_k \mathcal{A}_f(k) - \partial_k \mathcal{A}_s(k) \), where the integral is inside the mirror-symmetric plane. This is another example to use Green’s function to compute the topological index for HOTIs with interaction.

Higher-order topological phases can also be realized in superconductors. Our method based on Green’s function is applicable to higher-order topological superconductors as well. The Green’s function \( \mathcal{G} \) for superconductors includes both the particle-hole and particle-particle channels:
\[ \mathcal{G}(i\omega, k) = \begin{pmatrix} G_A(i\omega, k) & G_B(i\omega, k) \\ G_C(i\omega, k) & G_D(i\omega, k) \end{pmatrix}, \tag{15} \]
where

\[
(G_A)_{\alpha\beta}(i\omega, \mathbf{k}) = -\int_0^\beta d\tau e^{i\omega \tau} \left(T_{\tau} c_{\mathbf{k}\alpha}(\tau)^\dagger c_{\mathbf{k}\beta}(0)\right),
\]

\[
(G_B)_{\alpha\beta}(i\omega, \mathbf{k}) = -\int_0^\beta d\tau e^{i\omega \tau} \left(T_{\tau} c_{\mathbf{k}\alpha}(\tau)c_{-\mathbf{k}\beta}(0)\right),
\]

\[
(G_C)_{\alpha\beta}(i\omega, \mathbf{k}) = -\int_0^\beta d\tau e^{i\omega \tau} \left(T_{\tau} c_{-\mathbf{k}\alpha}(\tau)^\dagger c_{\mathbf{k}\beta}(0)\right),
\]

\[
(G_D)_{\alpha\beta}(i\omega, \mathbf{k}) = -\int_0^\beta d\tau e^{i\omega \tau} \left(T_{\tau} c_{-\mathbf{k}\alpha}(\tau)c_{-\mathbf{k}\beta}(0)\right).
\]

Then one can obtain the eigenstates of the inverse Green’s function at zero frequency

\[
\mathcal{G}^{-1}(0, \mathbf{k}) |g_n(\mathbf{k})\rangle = \lambda_n(\mathbf{k}) |g_n(\mathbf{k})\rangle,
\]

and $|g_n(\mathbf{k})\rangle$ can be utilized to compute the topological index. For interacting second-order topological superconductor protected by $C_4 T$ symmetry, the topological index can be computed via Eq.(12), and with an additional $S_4$ symmetry it can be computed via Eq.(14).

The $C_4 T$-symmetric second-order topological superconductor can be realized by $p + i d$ pairing as shown in Ref. 69:

\[
\hat{H} = \sum_k c_k^\dagger (\frac{k^2}{2m} - \mu) c_k + \Delta_p c_k^\dagger (\mathbf{k} \cdot \sigma)i\sigma_y c_{-\mathbf{k}} + \Delta_d c_k^\dagger (k_y^2 - k_x^2)i\sigma_x c_{-\mathbf{k}} + h.c.
\]

The lattice-regularized BdG Hamiltonian in the Nambu basis $\Psi_k = (c_{k\uparrow}, c_{k\downarrow}, c_{-k\downarrow}, c_{-k\uparrow})^T$ is given by:

\[
\hat{H}_k = \sum_{\mathbf{k}} \Psi_k^\dagger H_k \Psi_k,
\]

\[
H_k = (2t \cos(k_x a) + 2t \cos(k_y a) + 2t_z \cos(k_z c) - \mu) \tau_x \sigma_0 - \Delta_p \sin(k_x a) \tau_y \sigma_x + \Delta_d \sin(k_x a) \tau_x \sigma_y.
\]

Here $\tau$ is the particle-hole space and $\sigma$ is the spin space. Without the $d$-wave term $\Delta_d$, this Hamiltonian describes a first-order topological superconductor with $p$-wave pairing. It has time-reversal symmetry $T = -i\tau_0 \sigma_y K$, fourfold rotation symmetry $C_4 = \text{diag}(e^{i\pi/4}, e^{i\pi/4}, e^{i\pi/4}, e^{i\pi/4}) = 2^{-1/2}(\tau_0 \sigma_0 - \tau_z \sigma_z)$, and an effective “inversion” symmetry $I = \tau_z \sigma_0$ that satisfies $H_k I^\dagger = -H_k$. The $d$-wave term flips sign under $C_4, T, I$ symmetries separately but preserves the products $C_4 T$ and $S_4 = C_4 I$. The $d$-wave term also anti-commutes with the other terms in the Hamiltonian, hence it can open a surface gap to drive the system to a higher-order topological superconductor with chiral Majorana hinge states. Note that a $\pi/2$ phase difference between the $p$- and $d$-wave pairing is needed, otherwise the $d$-wave term will be $\tau_y \sigma_x$ instead which cannot open a surface gap. If we go beyond the mean-field level and take into account the quasiparticle interactions that are not included in Hamiltonian Eq.(19), the topological index cannot be computed from the wave functions obtained by diagonalization of the BdG Hamiltonian. Instead, it can be computed from the eigenstates of the inverse Green’s function $\mathcal{G}$ with the help of Eq.(12) or (14), similar to the case of higher-order topological insulators.

IV. NUMERICAL DEMONSTRATION OF THE GREEN’S FUNCTION APPROACH

We demonstrate the implementation of the Green’s function method by solving for the eigenstates of an interacting higher-order topological insulator via exact diagonalization (ED). The non-interacting part of the Hamiltonian is the same as Eq.(1), which describes a four-band 3D insulator with $C_4 T$ symmetry on a tetragonal lattice with two orbitals $A, B$ in each unit cell. The conduction and valence bands are separated by an energy gap $\Delta$. Denote the electron creation operator in the orbital space by $c_k^{\dagger s}$, where $s = A, B$. Then the creation operator for the $n$-th single particle band $\psi_k^{\dagger n}$ is related by $c_k^{\dagger s} = \sum_n \psi_k^{\dagger n}[u_n(\mathbf{k})]^T x_n$, where $u_n(\mathbf{k})$ is a four-component column vector for the $n$-th band of the single particle Hamiltonian $H_0$. Consider a repulsive Hubbard-like interaction:

\[
H_{int} = -\frac{U}{N_{cell}} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}, \ell} \epsilon_{\mathbf{k}q, \ell}^\dagger \epsilon_{\mathbf{k}'q, \ell}^\dagger [\psi_{\mathbf{k}q, \ell}^{\dagger}] [\psi_{\mathbf{k}'q, \ell}] .
\]

Here $N_{cell}$ is the number of unit cells. For simplicity we assume the interaction is local in momentum $k_z$. To perform exact diagonalization, we choose the basis of many-body states to have the form $|\Psi^{\text{basis}}\rangle = \prod_{\ell=1}^N [\psi_{\mathbf{k}q, \ell}^\dagger] x_n$, where $|0\rangle$ is the vacuum state and $N$ is the total number of electrons, which equals to the number of states in the valence bands $N = 2N_{cell}$. A generic many-body state $|\Psi\rangle$ is a superposition of different basis states. For each basis state $|\Psi^{\text{basis}}\rangle$, denote the number of electrons in the conduction bands by $N_c$. Then $N_c = 0$ corresponds to a unique state with all electrons filling up the valence bands, which is the ground state of single particle Hamiltonian. There are $N^2$ basis states with $N_c = 1$, corresponding to excitation obtained by moving an electron from the fully filled valence bands to conduction bands. Due to the energy gap $\Delta$, in the non-interacting limit the energy of the states with larger $N_c$ is higher than the ground state by at least $N_c \Delta$. Interaction can mix many-body states with different $N_c$ so that $N_c$ is no longer a good quantum number. However, for weak interaction $U \ll \Delta$ the many-body ground state should still mainly consist of states with small $N_c$. Therefore, in order to determine the ground state and Green’s function under weak interaction, it is sufficient to restrict the Hilbert space to many-body states with small $N_c$.

The computation of topological index $P_3$ involves $\mathcal{R}(k, k + G_0)$ in Eq.(12) where $k = (0, 0, k_z)$ and $G_0 = (\frac{a}{2}, \frac{a}{2}, 0)$. Denote the system size along $x$ and $y$ directions as $L \times L$. The minimal system size that can preserve the $C_4 T$ symmetry and make $\mathcal{R}(k, k + G_0)$ well-defined is $L = 4$. To keep the size of Hilbert space manageable, we only consider many-body states with $N_c = 0, 1, 2$ and focus on the weak and intermediate interaction region. $\mathcal{R}(k, k + G_0)$ depends only on $k_z$, hence we treat each $k_z$ independently and for a given $k_z$, the system
there is sizable difference between the two curves, indicating the many-body states with larger \( N_c \) need to be taken into account. We checked in a smaller system size \( L = 2 \) that including states with larger \( N_c \) does not qualitatively change the results. We performed full ED computation with all \( N_c \) included for \( L = 2 \) as shown in the grey curve in Fig.2(c). At large \( U \) the exact ground state is still non-degenerate and separated from the other states by an energy gap, and it has a sizable overlap with \( |\Psi^{\text{Bloch}}\rangle \). Therefore, for the \( L = 4 \) system the approximation of taking \( N_{c,\text{max}} = 2 \) still gives a valid description of the ground state if we focus on the weak interaction region.

The Green’s function can be computed via Lehmann representation:

\[
G_{\alpha\beta}(0, k) = \sum_m \frac{(\langle \Psi^g | c_{k\alpha} | \Psi_m \rangle \langle \Psi_m | c_{k\beta}^\dagger | \Psi_g \rangle)}{(E_m - E_g)} - \frac{(\langle \Psi_m | c_{k\alpha}^\dagger | \Psi_g \rangle \langle \Psi_g | c_{k\beta} | \Psi_m \rangle)}{(E_m - E_g)}. 
\]

Here \( \alpha, \beta \) represent combined indices for orbital and spin. \( |\Psi^g\rangle \) is the ground state with \( N \) electrons and \( |\Psi_m\rangle \) represents excited state with \( N \pm 1 \) electrons. Therefore, calculating the Green’s function for a \( N \)-particle system also requires ED computation for systems with \( N \pm 1 \) particles, which correspond to single-particle \( (N + 1) \) and single-hole \( (N - 1) \) excitation above the \( N \)-particle ground state. The spectrum for \( N \pm 1 \) particles is also shown in Fig.2(a) as the red signs, where only the lowest energy state is shown for each momentum.

We compute the Green’s function for systems with size \( L = 4 \) by Eq.(21). An effective Hamiltonian can be defined by \( H_{\text{eff}}(k) = -G(0, k)^{-1} \). In the non-interacting limit \( H_{\text{eff}} \) is the same as \( H_0 \), and with finite interaction \( H_{\text{eff}} \) changes but it still preserves the symmetries. As long as \( H_{\text{eff}} \) remains gapped, the quantity \( \mathcal{R}(k, \mathbf{k} + \mathbf{G}_0) \) is well-defined and can be used to compute the topological index. We calculate \( \mathcal{R}(k, \mathbf{k} + \mathbf{G}_0) \) where \( \mathbf{k} = (0, 0, k_z) \) using the eigenvectors of the inverse Green’s function. Denote the phase of \( \mathcal{R}(k, \mathbf{k} + \mathbf{G}_0) \) as \( \phi_{\mathbf{R}} \).

The evolution of \( \phi_{\mathbf{R}} \) as a function of \( k_z \) for \( U = 0.5\Delta \) and \( U = 0 \) systems are shown in Fig.2(d). In both cases the phase \( \phi_{\mathbf{R}} \) shows a winding \( 2\pi \) as \( k_z \) increases, hence by Eq.(12) the topological index \( P_3 \) is nontrivial for both systems. If interaction becomes stronger \( U \gtrsim \Delta \), the single-hole excitation energy can drop below the ground state energy, and the eigenvalues of the inverse Green’s function will cross zero. Then the effective Hamiltonian is no longer gapped, which leads to a topological transition out of the HOTI phase. Note that for the finite interaction \( U = 0.5\Delta \) in Fig.2(c,d) the effective Hamiltonian \( H_{\text{eff}} \) is still gapped and the topological index is well-defined. However, the many-body ground state is no longer a simple direct product state and the non-interacting formalism for topological indices are no longer applicable, but the Green’s function method still remains valid. Therefore, the Green’s function method is useful to identify the topological properties of interacting systems.
V. REALIZATION OF HIGHER-ORDER TOPOLOGICAL PHASES

The higher-order topological insulators protected by $C_4T$ symmetry discussed above can be generated by appropriate magnetic order that breaks time-reversal and fourfold rotation symmetries down to $C_4T$. Here we discuss some possible crystal structure and the corresponding magnetic order that can realize this phase.

Consider the lattice represented by the black sites in Fig.3(a),(b), where (a) and (b) are the top view and front view of the three dimensional lattice respectively. Suppose there is one orbital and one electron per site, and the unit cell contains two sites denoted by the green circle. The blue arrows represent magnetization on a different type of atoms. Without the blue arrows, the black sites form a lattice with $C_4$ symmetry along $z$ direction, inversion symmetry at the center of unit cell and time-reversal symmetry. With appropriate hopping amplitudes and spin-orbit coupling, electrons at the black sites can form a first-order topological insulator. We denote the hopping parameters in Fig.3(b) and choose the basis $\{c_A, c_A^\dagger, c_B, c_B^\dagger\}$ where $A, B$ represent the two sites in each unit cell. Up to an identity matrix that does not change the topology, the Hamiltonian is

$$H_{TT}(k) = (2t \cos(k_x a) + 2t \cos(k_y a) + 2t_z \cos(k_z c) + m) \times \tau_x \sigma_0 + \lambda \sin(k_x a) \tau_z \sigma_x + \lambda \sin(k_y a) \tau_z \sigma_y + 2t'_z \sin(k_z c) \tau_y \sigma_0.$$  

Here $\tau$ and $\sigma$ denote sublattices and spin spaces respectively. $t_z = (t_{z1} + t_{z2})/2, t'_z = (t_{z1} - t_{z2})/2$ and $\lambda$ is from spin-orbit coupling. This system has time-reversal symmetry $T = -i\tau_0 \sigma_0 K$, fourfold rotational symmetry $C_4 = \tau_0 e^{-i\pi/4} \sigma_z$ and inversion symmetry $I = \tau_x \sigma_0$. When $\max\{|4|t| - 2|t_z|, 2|t_z|\} < |m| < 4|t| + 2|t_z|$ it is a first-order topological insulator protected by time-reversal symmetry.

The presence of magnetization represented by the blue arrows breaks the symmetry into $C_4T$ and $S_4 = C_4I$. The hybridization between the states at the black and blue sites can modify the hopping amplitude between electrons on the black sites in a spin-dependent way. For example, for electrons hopping between two neighboring black sites, if the magnetization on the blue site in the middle of the hopping path is along $+z$ direction, then electrons with spin along $-z$ direction on one black site can hop to the middle blue site and then hop to the next black site, while for electrons on the black site with spin along $+z$ direction this hopping process mediated by the middle site is Pauli-blocked. Therefore, the presence of the magnetization in the hopping path can generate a spin-dependent hopping term proportional to $\sigma_z$. From the magnetic order in Fig.3(a), the magnetization that surrounds electrons on black sites is positive along $\pm x$ direction and negative along $\pm y$ direction, and from Fig.3(b) the magnetization around the two sublattices is opposite, this magnetic order generates a new term $(\cos(k_x a) - \cos(k_y a)) \tau_z \sigma_z$ so that the Hamiltonian with magnetic order becomes

$$H_{HOT}(k) = H_{TT}(k) + \Delta_2 (\cos(k_x a) - \cos(k_y a)) \tau_z \sigma_z.$$  

Eq.(23) is equivalent to the higher-order topological insulator in Eq.(1) up to a unitary transformation. Therefore the magnetic order drives the system into a higher order topological insulator protected by $C_4T$ symmetry. The pattern of magnetization also indicates the system has an additional $S_4$ symmetry.

The $C_4T$-symmetric higher-order topological insulator can also be realized in the lattice denoted by Fig.3(a),(c). Here each unit cell has one black site and each site has one $s$-type and one $p_\perp$-type orbitals. Band inversion can occur between bands generated by the even- and odd-parity orbitals, leading to a first-order topological insulator. The magnetic order modifies the hopping amplitude between electrons on black sites by adding hopping terms proportional to $\pm \sigma_z$ similar to the above analysis. These spin-dependent hopping terms break time-reversal symmetry. Because the magnetic order preserves $C_4T$ symmetry, the hopping terms it generates also preserve $C_4T$, which drives the system to $C_4T$-protected higher-order topological insulator. Contrary to the magnetic order given by Fig.3(a),(b), the lattice (a),(c) preserves inversion symmetry and breaks $S_4$ symmetry.

The lattice in Fig.3(a),(b) can be realized in the crystal structures in Fig.4(a). This structure can be viewed as a variation of antiperovskite structure $ABX_3$ with the top $X$ ion replaced by a different type of element, and the $c$ axis can acquire a lattice constant different from the $ab$ plane. If the bands close to Fermi level are from the B sites in the center, and a Neel order indicated by the blue arrows is developed surrounding the B sites, this structure can reproduce the physics in Fig.3(a),(b) to realize a higher-order topological insulator protected by $C_4T$ symmetry. Similarly, the lattice in Fig.3(a),(c) can be realized by the magnetic order in Fig.4(b). The active electrons can also sit on body-centered tetragonal Bravais lattice as in the anti-ruddlesden-popper structure in Fig.4(c). If the active electrons are on the red sites in the center, the in-plane antiferromagnetic ordering indicated by the blue arrows breaks time-reversal but preserves $C_4T$ and can drive the system into a higher-order topological insulator.

The Coulomb interaction is ubiquitous in real materials. If Coulomb interaction is taken into account, the ground state is no longer a simple direct product of Bloch states but the higher-
order topological features still persist for weak interaction. For the interacting system we can go through a procedure similar to Sec. IV and use the eigenstates of inverse Green’s function and the symmetry operators to compute the topological index via Eq.(12) or Eq.(14).

VI. STABILITY OF HIGHER-ORDER TOPOLOGICAL PHASES

When the higher-order topological index for an interacting system is nontrivial, gapless hinge modes are expected to emerge from bulk-boundary correspondence. In this section we discuss the stability of these hinge modes against Coulomb interaction in the bulk and deformation at the boundary, and show that a finite surface gap is crucial to ensure the stability of these hinge modes.

A. Stability against Coulomb interaction

Higher-order topological insulators have an energy gap in both the bulk and surface. If perturbations are added to the system, it is generally expected that as long as the perturbations are not strong enough to make the gap vanish, the higher-order topological phase should be robust. However, there is a recent debate in the literature on whether this HOTI phase is stable under Coulomb interaction. In particular, Refs. 64 and 66 use the renormalization group and conclude that an infinitesimal long-ranged Coulomb interaction can destroy the HOTI phase. On the other hand, Ref. 65 argues that it is stable against a weak Coulomb interaction due to a different criterion for the stability. In order to test these claims, we perform a ED computation by adding a weak long-ranged interaction \( H_V \) as well as the Hubbard-like interaction in Eq.(20) to the free HOTI Hamiltonian in Eq.(1):

\[
H_V = \sum_{i \neq j, \alpha \beta} V_{ij} c_{i \alpha}^{\dagger} c_{i \alpha}^{\dagger} c_{j \beta} c_{j \beta}, \quad V_{ij} = \frac{V_0}{r_{ij}}.
\]

Here \( i, j \) label the location of unit cell, \( r_{ij} \) is the distance between \( i \) and \( j \) in units of nearest neighbor distance, and \( \alpha, \beta \) are combined orbital and spin indices. We computed the Green’s function and the phase \( \phi_R \) of \( \mathcal{R}(\mathbf{k}, \mathbf{k} + \mathbf{G}_0) \) under weak interaction \( U = 0.2 \) and \( V_0 = 0.01 \) and find that \( \phi_R \) still shows a winding with \( k_z \) as shown in Fig.5, indicating a nontrivial topological index. This suggests a weak interaction cannot lead to a transition to the trivial phase, which is in agreement with Ref. 65.

B. Stability against boundary deformation

The gapless hinge modes emerge as features indicating the higher-order topology. This nomenclature seems to suggest the requirement of a sharp hinge at the boundary, and it raises a natural question as to whether these hinge modes still exist if the boundary does not have a sharp hinge. In addition, the bulk-boundary correspondence (BBC) for symmetry-protected higher-order topological phases usually requires the set of boundaries to preserve the same symmetry, e.g., the four side surfaces in Fig.1(a) for the model in Eq.(1) need to be related to each other by fourfold rotational symmetry. This is because the hinge is the direct boundary of 2D surfaces rather than the 3D bulk. If 2D surfaces are allowed to break the symmetry, one can annihilate the hinge states without closing the 3D bulk gap. In reality the crystalline symmetry can be easily broken by the boundary truncation, and it is natural to ask whether these hinge modes still exist. In this section we aim to answer whether the existence of hinge states requires the boundaries as a whole to preserve the symmetry, and whether it requires the boundary to have a sharp physical hinge. We show that neither of these conditions are necessary for the hinge states to appear.

Consider a sample that microscopically realizes a higher-order topological insulator, e.g., the model in Eq.(1) and possibly with interactions, but has the macroscopic shape of a cylinder with axis along \( z \) direction, instead of the cubic shape in Fig.1(a). If there is no \( \Delta_2 \) term, the system is a first-order topological insulator and the effective Hamiltonian on the side...
The emergence of these effective hinge states can be understood by linearly expanding the surface Hamiltonian near \( \phi = \pm \frac{\pi}{4}, \pm \frac{3\pi}{4} \) where the surface mass changes sign. Let \( x \) denote the spatial coordinate along \( \phi \) direction, Eq.(27) reduces to

\[
\left( \pm \frac{2m_x}{R} - \frac{i}{R} \frac{\partial}{\partial \phi} \right) a(x) + \left( -i \frac{\partial}{\partial \phi} \right) b(x) = E \left( a(\phi) \right).
\]

This equation can be solved by expanding \( a(\phi) \) and \( b(\phi) \) in terms of \( e^{\pm i \phi} \). The solution shows that for large \( R \) there are four eigenstates with zero energy located at \( \phi = \pm \frac{\pi}{4}, \pm \frac{3\pi}{4} \), as in Fig.6(a),(b). These eigenstates are close to Gaussian functions of \( \phi \) and are spatially separated. The small angular width \( \Delta \phi \) and the extended nature along \( z \) direction make these eigenstates effectively "hinge states" although the cylindrical boundary has no hinge.

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\]
of the hinge state will increase and occupy the whole surface when the surface becomes flat. This is consistent with the fact that the surface mass term $m_1 \cos 2\phi$ can gap out the surfaces perpendicular to $x$ or $y$ directions but not the surfaces perpendicular to $s + y$, where $x$ and $y$ directions are along crystalline axes corresponding to $\phi = 0$ and $\phi = \pi/2$ respectively.

To verify these predictions obtained from the effective surface Hamiltonian, we diagonalize the tight-binding model in Eq.(1) on a finite-size system with the shape of one-quarter cylinder in Fig.7. The $z$ direction is taken to be periodic. We find that at $k_z = 0$, there are four eigenstates with zero energy, with three of them localized at the hinges, and one localized at cylindrical part of the surface. We use Gaussian fit $|\psi|^2 = A \exp(-\frac{x^2}{2\sigma^2})$ to obtain the width of the state at the cylindrical surface, as shown in the inset of Fig.7. Here $x$ is the distance to the center of the zero mode. Define width $w$ by the location where the Gaussian curve reduces to half its peak value, then $w = 2.35\sigma$. The fitting shows the wave function profile approaches a Gaussian function when $R$ increases, while for small $R = 40$ there is deviation from Gaussian due to finite size effect. For $R = 40$ and 80 we obtain $w = 16.6$ and 20.6 respectively. $w^2$ as a function of $R$ in various system sizes is shown in Fig.7(c). The linear relation between $w^2$ and $R$ indicates $w \sim \sqrt{R}$ and $\Delta \Phi \sim 1/\sqrt{R}$ at large system size. Therefore, as the system size increases, the angular width $\Delta \Phi$ of the state at the cylindrical surface decreases, approaching an effective hinge state. Therefore, the emergence of hinge states as features of higher-order topology does not require the boundaries to preserve the protecting symmetry nor does it require the existence of a physical hinge. Although the computation in Fig.7 is performed for a non-interacting system, the hinge modes are expected to persist under weak interaction due to the presence of a finite surface gap. However, a direct numerical verification of the existence of hinge states in an interacting system with large system size is beyond the scope of this work.

We emphasize that the above conclusions do not imply these hinge states will emerge under arbitrary boundary conditions that break the protecting symmetry. For example, due to the absence of $C_4T$ symmetry on the boundary, in principle the hinge states in Fig.1(a) can be removed by superimposing a layer of Chern insulator to the left and right side surfaces respectively. However, this process has to be a large perturbation that closes the surface gap. Our results in Fig.6 and 7 show that if the boundary is obtained by truncating the crystal rather than decorating with another material, then the presence of hinge states is a local property of the boundary, independent of whether the boundary satisfies the global symmetry. In regards of the realization of these hinge states in experiments, this implies the boundary termination of the sample does not need to strictly obey the symmetry and does not require a sharp hinge for these hinge states to be observed.

VII. CONCLUSION

We show that the eigenstates of inverse Green’s function at zero frequency are useful tools in characterizing higher-order topological phases with electronic interaction. In particular, it enables us to compute the topological index of interacting $C_4T$-symmetric second-order topological insulator in a gauge-independent way, and with additional $S_4$ symmetry the topological index the interacting system can be determined by $S_4$ eigenvalues directly, similar to the Fu-Kane formula. This Green’s function-based approach can also be applied to compute the topological index for higher-order topological superconductors. We demonstrate that the hinge states as features of higher-order topology are robust to interaction and deformation of boundaries. If the sample of higher-order topological insulator is sufficiently large and has natural open boundary condition such that its boundaries are obtained by truncating the crystal, the hinge states survive even in the absence of a physical hinge at the boundary. We also propose crystal structures with $C_4T$-preserving magnetic order as possible platforms to realize this higher-order topological phase with electron interactions.

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Appendix A: Details in the derivation of topological indices

1. Proof of anti-symmetry

The Pfaffian formula Eq.(8) requires the matrix $M$ to be anti-symmetric. We show that $M(k)$ is anti-symmetric for every $C_4$-invariant $k$ point such that $C_4Tk = C_4^{-1}Tk = -k$.

Let $\Theta = \frac{C_4T + C_4^{-1}T}{\sqrt{2}}$, we can show that $\Theta^2 = T^2 = -1$. This is due to $(C_4)^4 = (C_2)^2 = -1$, then $C_2 + C_2^{-1} = 0$ and $\Theta^2 = -(C_4 + C_4^{-1})^2/2 = -(C_2 + C_2^{-1} + 2)/2 = -1$. Therefore $\Theta$ is an anti-unitary operator similar to the time-reversal operator for spin 1/2 systems which gives rise to Kramers degeneracy. Then for every $C_4$-invariant momentum $k$ we have

$$M_{nm}(k) = \langle g_m(k) | \Theta | g_n(k) \rangle = \langle \Theta^2 g_n(k) | \Theta | g_m(k) \rangle = -\langle g_n(k) | \Theta | g_m(k) \rangle = -M_{nm}(k). \quad (S1)$$

This shows $M(k)$ is anti-symmetric, hence its Pfaffian is well-defined.

2. Proof of Eq.(12)

We present the derivation that leads to Eq.(12) in the main text. This part follows Ref. 68. First we show that the
line quantity $\mathcal{R}$ in Eq.(10) is gauge-invariant, i.e., invariant under gauge transformation $|g_n(k)| \rightarrow \sum_m |g_m(k)|U_{mn}(k)$ where $U$ is a unitary matrix and the summation is over the eigenstates of inverse Green’s function with positive eigenvalues. First consider the limit in which $k_1$ and $k_2$ are close to each other. Then $W(k_1, k_2) = (g_m(k_1)|g_n(k_2))$. Under the gauge transformation, $M_{mn}(k) = \langle g_m(k)|g_n(k)\rangle \rightarrow (U(k)^\dagger M(k)U(k^2))_{mn}$, $W_{mn}(k_1, k_2) = (g_m(k_1)|g_n(k_2)) \rightarrow (U(k)^\dagger W(k_1, k_2)U(k^2))_{mn}$. Therefore

$$\text{det}(W(k_1, k_2)) \rightarrow \text{det}(W(k_1, k_2)) \text{det}(U(k))^{-1} \text{det}(U(k^2)) = \mathcal{R}(k_1, k_2).$$

This shows that $\mathcal{R}(k_1, k_2)$ is gauge-invariant when $k_1$ is close to $k_2$. For a general pair of separated momentum points $k_1$ and $k_2$, we can divide the path connecting $k_1$, $k_2$ by small segments $(k_1, k_{i+1})$. Then $\mathcal{R}(k_a, k_b) = \prod_i \mathcal{R}(k_i, k_{i+1})$. For each small segment $\mathcal{R}(k_i, k_{i+1})$ is gauge-invariant, therefore $\mathcal{R}(k_a, k_b)$ is gauge-invariant as well. This gauge-invariance allows us to compute $\mathcal{R}$ without a smooth gauge.

Next we show that $\mathcal{R}$ can be related to the topological index $P_3$. Select a gauge on the straight line $ZZ'$ such that $|g_n(k)|$ is smooth and periodic. For each $k = (k_x, k_y, k_z)$ in the region $\tau_{1/2}$ in Fig.1(b), let $k_p = (0, 0, k_z)$ and then a parallel transport gauge that is smooth in $\tau_{1/2}$ can be defined by

$$|g_m(k)| = \prod_{k_p \in \mathbb{Z}} P_{k_p} |g_m(k_p)|. \quad (S2)$$

In this gauge for each $k \in ZZ'$, $\text{det}(W(k, k + G_0))$ becomes unity, and we get

$$\mathcal{R}(k, k + G_0) = \frac{\text{det}(|M(k + G_0)|)}{\text{det}(|M(k)|)}. \quad (S3)$$

Note that $k + G_0 \in AA'$ if $k \in ZZ'$. Therefore, Eq.(12) becomes the winding of the phase of $\text{det}(W(k, k + G_0))$ along $ZZ'$ and $AA'$, which is equivalent to $\hat{\tau}_{1/2}$ since contribution along $ZA$ and $Z'Z'$ cancel by periodicity. Therefore, Eq.(12) represents the winding of Pfaffian along $\hat{\tau}_{1/2}$, which is equivalent to Eq.(8). This proves Eq.(12) in the parallel transport gauge. Because $\mathcal{R}$ is gauge-invariant, Eq.(12) should be true in any gauge. This finishes the proof.

The advantage of Eq.(12) is that because $\mathcal{R}$ is gauge-invariant, the construction of the smooth parallel transport gauge in Eq.(S2) is not needed in actual computation. In practice one can evaluate Eq.(12) in any gauge obtained by diagonalizing the inverse Green’s function.

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1 Xiao-Liang Qi and Shou-Cheng Zhang, “Topological insulators and superconductors,” Rev. Mod. Phys. 83, 1057–1110 (2011).
2 Xiao-Liang Qi, Taylor L. Hughes, and Shou-Cheng Zhang, “Topological field theory of time-reversal invariant insulators,” Phys. Rev. B 78, 195424 (2008).
3 M. Z. Hasan and C. L. Kane, “Colloquium: Topological insulators,” Rev. Mod. Phys. 82, 3045–3067 (2010).
4 Liang Fu and C. L. Kane, “Time reversal polarization and a $Z_2$ adiabatic spin pump,” Phys. Rev. B 74, 195312 (2006).
5 Liang Fu, C. L. Kane, and E. J. Mele, “Topological insulators in three dimensions,” Phys. Rev. Lett. 98, 106803 (2007).
6 Liang Fu and C. L. Kane, “Topological insulators with inversion symmetry,” Phys. Rev. B 76, 045302 (2007).
7 C. L. Kane and E. J. Mele, “$Z_2$ topological order and the quantum spin hall effect,” Phys. Rev. Lett. 95, 146802 (2005).
8 Wladimir A. Benalcazar, B. Andrei Bernevig, and Taylor L. Hughes, “Quantized electric multipole insulators,” Science 357, 61–66 (2017).
9 Wladimir A. Benalcazar, B. Andrei Bernevig, and Taylor L. Hughes, “Electric multipole moments, topological multipole moment pumping, and chiral hinge states in crystalline insulators,” Phys. Rev. B 96, 245115 (2017).
10 Frank Schindler, Ashley M. Cook, Maia G. Vergniory, Zhijun Wang, Stuart S. Parkin, B. Andrei Bernevig, and Titus Neupert, “Higher-order topological insulators,” Sci. Adv 4 (2018), 10.1126/sciadv.aat0346.
11 Junyeeong Ahn and Bohm-Jung Yang, “Symmetry representation approach to topological invariants in $C_{2v}$-symmetric systems,” Phys. Rev. B 99, 235125 (2019).
12 Benjamin J. Wieder and B. Andrei Bernevig, “The Axion Insulator as a Pump of Fragile Topology,” arXiv:1810.02373.
13 Motohiko Ezawa, “Strong and weak second-order topological insulators with hexagonal symmetry and $F_3$ index,” Phys. Rev. B 97, 241402 (2018).
14 Motohiko Ezawa, “Magnetic second-order topological insulators and semimetals,” Phys. Rev. B 97, 155305 (2018).
15 Chen Fang and Liang Fu, “New classes of three-dimensional topological crystalline insulators: Nonsymmorphic and magnetic,” Phys. Rev. B 91, 161105 (2015).
16 Guido van Miert and Carmine Ortix, “Higher-order topological insulators protected by inversion and rotoinversion symmetries,” Phys. Rev. B 98, 081110 (2018).
17 Eslam Khalaf, “Higher-order topological insulators and superconductors protected by inversion symmetry,” Phys. Rev. B 97, 205136 (2018).
18 Sander H. Kooi, Guido van Miert, and Carmine Ortix, “Inversion-symmetry protected chiral hinge states in stacks of doped quantum hall layers,” Phys. Rev. B 98, 245102 (2018).
19 Dumitru Călugăru, Vladimir Juričić, and Bitan Roy, “Higher-order topological phases: A general principle of construction,” Phys. Rev. B 99, 041301 (2019).
20 Dániel Varjas, Fernando de Juan, and Yuan-Ming Lu, “Bulk invariants and topological response in insulators and superconductors with nonsymmorphic symmetries,” Phys. Rev. B 92, 195116 (2015).
21 Motohiko Ezawa, “Second-order topological insulators and loop-nodal semimetals in transition metal dichalcogenides $\text{XTe}_2$ ($X = \text{Mo, W}$),” Sci. Rep 9, 5286 (2019).
22 Zhijun Wang, Benjamin J. Wieder, Jian Li, Binghai Yan, and B. Andrei Bernevig, “Higher-order topology, monopole nodal
lines, and the origin of large fermi arcs in transition metal dichalcogenides \( x \text{Se}_2 \) (\( x = \text{Mo, W} \))." Phys. Rev. Lett. 123, 186401 (2019).

23 Zhida Song, Zhong Fang, and Chen Fang, "(d - 2)-dimensional edge states of rotation symmetry protected topological states," Phys. Rev. Lett. 119, 246402 (2017).

24 Akishi Matsugatani and Haruki Watanabe, "Connecting higher-order topological insulators to lower-dimensional topological insulators," Phys. Rev. B 98, 205129 (2018).

25 Josias Langbehn, Yang Peng, Luka Trifunovic, Felix von Oppen, and Piet W. Brouwer, "Reflection-symmetric second-order topological insulators and superconductors," Phys. Rev. Lett. 119, 246401 (2017).

26 Changming Yue, Yuanfeng Xu, Zhida Song, Hongming Weng, Yuan-Ming Lu, Chen Fang, and Xi Dai, "Symmetry-enforced chiral hinge states and surface quantum anomalous hall effect in the magnetic axion insulator bi2-xmxse3," Nat. Phys. 15, 577–581 (2019).

27 Chen-Hsuan Hsu, Peter Stano, Jelena Klinovaja, and Daniel Loss, "Majorana kramers pairs in higher-order topological insulators," Phys. Rev. Lett. 121, 196801 (2018).

28 Raquel Queiroz and Ady Stern, "Splitting the hinge mode of higher-order topological insulators," Phys. Rev. Lett. 123, 036802 (2019).

29 Haoran Xue, Yahui Yang, Fei Gao, Yidong Chong, and Baile Zhang, "Acoustic higher-order topological insulator on a kagome lattice," Nat. Mater. 18, 108–112 (2019).

30 Max Geier, Luka Trifunovic, Max Hoskam, and Piet W. Brouwer, "Second-order topological insulators and superconductors with an order-two crystalline symmetry," Phys. Rev. B 97, 205135 (2018).

31 Frank Schindler, Zhijun Wang, Maia G. Vergniory, Ashley M. Cook, Anil Murani, Shamashis Sengupta, Alik Yu Kasumov, Richard Debloock, Sangjun Jeon, Ilya Drozdov, Hélène Bouchiat, Sophie Guérin, Ali Yazdani, B. Andrei Bernevig, and Titus Neupert, "Higher-order topology in bismuth," Nat. Phys. 14, 918–924 (2018).

32 Luka Trifunovic and Piet W. Brouwer, "Higher-order bulk-boundary correspondence for topological phase transitions," Phys. Rev. X 9, 011012 (2019).

33 Sayed Ali Akbar Ghorashi, Xiang Hu, Taylor L. Hughes, and Enrico Rossi, "Second-order dirac superconductors and magnetic field induced majorana hinge modes," Phys. Rev. B 100, 020509 (2019).

34 Tanay Nag, Vladimir Juričić, and Bitan Roy, "Hierarchy of higher-order floquet topological phases in three dimensions," Phys. Rev. B 103, 115308 (2020).

35 Arnob Kumar Ghosh, Tanay Nag, and Arjitt Saha, "Hierarchy of higher-order topological superconductors in three dimensions," Phys. Rev. B 104, 134508 (2021).

36 Luka Trifunovic and Piet W. Brouwer, "Higher-order topological band structures," physica status solidi (b) 258, 2000090 (2021).

37 Wladimir A. Benalcazar, Tianhe Li, and Taylor L. Hughes, "Quantization of fractional corner charge in \( C_n \)-symmetric higher-order topological crystalline insulators," Phys. Rev. B 99, 245151 (2019).

38 Yuan Fang and Jennifer Cano, "Filling anomaly for general two- and three-dimensional \( C_4 \) symmetric lattices," Phys. Rev. B 103, 165109 (2021).

39 Wonjun Lee, Gil Young Cho, and Byungmin Kang, "Many-body quadrupolar sum rule for higher-order topological insulators," Phys. Rev. B 105, 155143 (2022).

40 Rui Yu, Xiao Liang Qi, Andrei Bernevig, Zhong Fang, and Xi Dai, "Equivalent expression of \( F_2 \) topological invariant for band insulators using the non-abelian berry connection," Phys. Rev. B 84, 075119 (2011).

41 S. Franca, J. van den Brink, and I. C. Fulga, "An anomalous higher-order topological insulator," Phys. Rev. B 98, 201114 (2018).

42 Adrien Bouhon, Annica M. Black-Schaffer, and Robert-Jan Slager, "Wilson loop approach to fragile topology of split elementary band representations and topological crystalline insulators with time-reversal symmetry," Phys. Rev. B 100, 195135 (2019).

43 Chen Fang, Matthew J. Gilbert, and B. Andrei Bernevig, "Bulk topological invariants in noninteracting point group symmetric insulators," Phys. Rev. B 86, 115112 (2012).

44 Barry Bradlyn, L. Elcoro, Jennifer Cano, M. G. Vergniory, Zhijun Wang, C. Felser, M. I. Aroyo, and B. Andrei Bernevig, "Topological quantum chemistry," Nature 547, 298 EP – (2017).

45 Hoi Chun Po, Ashvin Vishwanath, and Haruki Watanabe, "Symmetry-based indicators of band topology in the 230 space groups," Nat. Commun. 8, 50 (2017).

46 Jorrit Kruthoff, Jan de Boer, Jasper van Wezel, Charles L. Kane, and Robert-Jan Slager, "Topological classification of crystalline insulators through band structure combinatorics," Phys. Rev. X 7, 041069 (2017).

47 Eslam Khalaf, Hoi Chun Po, Ashvin Vishwanath, and Haruki Watanabe, "Symmetry indicators and anomalous surface states of topological crystalline insulators," Phys. Rev. X 8, 031070 (2018).

48 Seishiro Ono and Haruki Watanabe, "Unified understanding of symmetry indicators for all internal symmetry classes," Phys. Rev. B 98, 115150 (2018).

49 Zhida Song, Tiantian Zhang, Zhong Fang, and Chen Fang, "Quantitative mappings between symmetry and topology in solids," Nature Communications 9, 3530 (2018).

50 Tiantian Zhang, Yi Jiang, Zhida Song, He Huang, Yuqing He, Zhong Fang, Hongming Weng, and Chen Fang, "Catalogue of topological electronic materials," Nature 566, 475–479 (2019).

51 Feng Tang, Hoi Chun Po, Ashvin Vishwanath, and Xiangang Wan, "Comprehensive search for topological materials using symmetry indicators," Nature 566, 486–489 (2019).

52 M. G. Vergniory, L. Elcoro, Claudia Felser, Nicolas Regnault, B. Andrei Bernevig, and Zhijun Wang, "A complete catalogue of high-quality topological materials," Nature 566, 480–485 (2019).

53 Lukasz Fidkowski and Alexei Kitaev, "Effects of interactions on the topological classification of free fermion systems," Phys. Rev. B 81, 134509 (2010).

54 Raffaele Resta, "Quantum-mechanical position operator in extended systems," Phys. Rev. Lett. 80, 1800–1803 (1998).

55 Robert-Jan Slager, Louk Rademaker, Jan Zaanen, and Leon Balents, "Impurity-bound states and green’s function zeroes as local signatures of topology," Phys. Rev. B 92, 085126 (2015).

56 Ken Shiozaki, Hassan Shapourian, Kiyonori Gomi, and Shinsei Ryu, "Many-body topological invariants for fermionic short-range entangled topological phases protected by antiunitary symmetries," Phys. Rev. B 98, 035151 (2018).

57 Byungmin Kang, Ken Shiozaki, and Gil Young Cho, "Many-body order parameters for multipoles in solids," Phys. Rev. B 100, 245134 (2019).

58 William A. Wheeler, Lucas K. Wagner, and Taylor L. Hughes, "Many-body electric multipole operators in extended systems," Phys. Rev. B 100, 245135 (2019).

59 Koji Kudo, Haruki Watanabe, Toshikaze Kariyado, and Yasuhiro Hatsugai, "Many-body chern number without integration," Phys. Rev. Lett. 122, 146601 (2019).

60 Byungmin Kang, Wonjun Lee, and Gil Young Cho, "Many-body invariants for chern and chiral hinge insulators," Phys. Rev. Lett. 126, 016402 (2021).

61 Zhong Wang, Xiao-Liang Qi, and Shou-Cheng Zhang, "Topological invariants for interacting topological insulators with inversion
symmetry,” *Phys. Rev. B* **85**, 165126 (2012).
62 Zhong Wang and Shou-Cheng Zhang, “Simplified topological invariants for interacting insulators,” *Phys. Rev. X* **2**, 031008 (2012).
63 Zhong Wang and Shou-Cheng Zhang, “Strongly correlated topological superconductors and topological phase transitions via green’s function,” *Phys. Rev. B* **86**, 165116 (2012).
64 Peng-Lu Zhao, Xiao-Bin Qiang, Hai-Zhou Lu, and X. C. Xie, “Coulomb instabilities of a three-dimensional higher-order topological insulator,” *Phys. Rev. Lett.* **127**, 176601 (2021).
65 Yu-Wen Lee and Min-Fong Yang, “Comment on “coulomb instabilities of a three-dimensional higher-order topological insulator”,” arXiv:2202.01642.
66 Jing-Rong Wang and Chang-Jin Zhang, “Fate of higher-order topological insulator under coulomb interaction,” arXiv:2202.03417.
67 Heqiu Li and Kai Sun, “Pfaffian formalism for higher-order topological insulators,” *Phys. Rev. Lett.* **124**, 036401 (2020).
68 Heqiu Li and Kai Sun, “Topological insulators and higher-order topological insulators from gauge-invariant one-dimensional lines,” *Phys. Rev. B* **102**, 085108 (2020).
69 Yuxuan Wang, Mao Lin, and Taylor L. Hughes, “Weak-pairing higher order topological superconductors,” *Phys. Rev. B* **98**, 165144 (2018).
70 Alexey A. Soluyanov and David Vanderbilt, “Smooth gauge for topological insulators,” *Phys. Rev. B* **85**, 115415 (2012).