Pfaffian Formalism for Higher-Order Topological Insulators

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We generalize the Pfaffian formalism, which has been playing an important role in the study of time-reversal invariant topological insulators (TIs), to 3D chiral higher-order topological insulators (HOTIs) protected by the product of fourfold rotational symmetry C_4 and the time-reversal symmetry T. This Pfaffian description reveals a deep and fundamental link between TIs and HOTIs, and allows important conclusions about TIs to be generalized to HOTIs. As examples, we demonstrate in the Letter how to generalize Fu-Kane's parity criterion for TIs to HOTIs, and also present a general method to efficiently compute the Z_2 index of 3D chiral HOTIs without a global gauge.

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Introduction.—In comparison to the well-studied topological insulators (TIs), which have a gapped d-dimensional bulk and topologically protected gapless states on its $d-1$ dimensional boundaries [1–7], the recently proposed higher-order topological insulators (HOTIs) have a similar gapped bulk, but the gapless states emerge at lower dimensions [8–30], e.g., the 1D hinge of a 3D insulator. In this Letter, we focus on second-order topological insulators characterized by nontrivial magnetoelectric polarization P_3, e.g., 3D chiral second-order topological insulators (CSOTIs) with gapless chiral hinge states propagating in alternative directions. The physical meaning of this topological invariant can be understood by the theory of electric multipole moments [8,9]. These second-order TIs have a strong connection to TIs, and, in particular, if the time-reversal symmetry T is enforced, $2P_3$ recovers the Z_2 index of a TI [31]. If the time-reversal symmetry is broken, $2P_3$ still defines a Z_2 topological index, as long as a space inversion, rotoinversion, or C_nT symmetry is preserved [10–17,32,33], where C_n represents n-fold rotation with $n=2$, 4, 6, and this Z_2 index, in the absence of time-reversal symmetry, characterizes a second-order TI. For systems invariant under space inversion or some rotoinversion, this topological index is fully dictated by high-symmetry momenta [34–39]. However, in general, the diagnosis of higher-order topology requires more sophisticated techniques like the nested Wilson loops [8–10,40–42].

Although TIs and these second-order TIs are characterized by the same P_3, which suggests a strong and deep connection between the two, one important link between TIs and second-order TIs is still missing, i.e., the Pfaffian formula for TIs developed by Fu and Kane [4]. This Pfaffian formula laid the foundation for many other important conclusions about TIs. For example, in principle, to compute the Z_2 index for a TI, it requires global information about the entire Brillouin zone (BZ). In practice, this means that a global gauge will be needed, such that wave functions are globally smooth and continuous in the entire Brillouin zone. Although the existence of such a gauge is guaranteed, finding it is not always straightforward. Based on the Pfaffian formula, several shortcuts were developed to bypass this complicated procedure of finding a global gauge, such as Fu-Kane's high-symmetry point approach for systems with space-inversion symmetry [4], and numerical techniques by Fukui and Hatsugai [43] and by Soluyanov and Vanderbilt [44], which dramatically reduced the computational costs. For second order TIs, however, due to the broken time-reversal symmetry, a Pfaffian formalism is still absent, and thus knowledge that we accumulated from studying TIs cannot be directly generalized.

In this Letter, we develop a Pfaffian formalism for higher-order topological insulators, more precisely CSOTIs, utilizing a composite operator obtained from the C_4T sewing matrix. We find that in strong analogy to TIs, the topological index of CSOTIs can also be determined via a Pfaffian formula. This conclusion not only provides a new pathway for computing topological indices, but also makes it possible to generalize existing Pfaffian-based knowledge about TIs to high-order TIs, such as methods to obtain topological indices without a global gauge. As examples, we will show below that our Pfaffian formula provides a straightforward generalization of the Fu-Kane's parity criterion [6] to second order TIs if a fourfold rotoinversion symmetry is present, which demonstrates a direct connection between P_3 and symmetry indicators [36,38]. For general CSOTIs without rotoinversion symmetry, our Pfaffian formalism indicates that high symmetry points alone do not contain sufficient information to fully dictate the topological index, but the Pfaffian formalism allows us to get the index through examining only a small part of the Brillouin zone without using a global gauge, along a similar line as what has been achieved for TIs [43,44].

Generalization of the Pfaffian formalism.—We consider a CSOTI invariant under C_4T but without T or C_4 symmetry,

and we set the rotational axis to be aligned with the z direction. The more generic systems will be covered in the discussion. The half-integer spin leads to $(C_4T)^4 = -1$, instead of $(C_4T)^2 = -1$, which has been studied in Ref. [45]. Because of the anti-unitary nature of C_4T and the half-integer spin of fermions, in analogy to Kramers doublets, all bands in our system shall show twofold degeneracy at C_4T-invariant momenta, denoted as $K^4 = \{\Gamma, M, Z, A\}$, where $\Gamma = (0,0,0)$, $M = (\pi,\pi,0)$, $Z = (0,0,\pi)$, $A = (\pi,\pi,\pi)$. Without losing generality, we assume that there is no accidental degeneracy beyond what is required by these Kramers pairs, because accidental degeneracy can always be lifted by perturbations without changing topological indices. Thus, for a system with $2N$ valance bands, a $2N \times 2N$ unitary sewing matrix for the symmetry operator C_4T can be defined:

$$B_{mn}(\mathbf{k}) = \langle u_m(C_4T\mathbf{k})|C_4T|u_n(\mathbf{k})\rangle, \tag{1}$$

where m, n are valence band indices, $C_4T\mathbf{k} \equiv (k_y, -k_x, -k_z)$, and $|u_n(\mathbf{k})\rangle$ is the periodic part of the Bloch wave function. In the absence of accidental degeneracy as assumed above, this $B(\mathbf{k})$ matrix is 2×2 block diagonal due to the Kramers pairs, i.e., $B = \mathrm{diag}(B_1, B_2, \ldots, B_N)$ with B_r's being 2×2 unitary matrices for $r = 1, 2, \ldots, N$. According to Ref. [31], there must exist a smooth gauge in our system such that $B_r(\mathbf{k})$ is globally smooth and $\det[B_r(\mathbf{k})] = 1$. Therefore as a function of momentum, each $B_r(\mathbf{k})$ defines a smooth mapping from the 3D BZ to the linear space formed by all $SU(2)$ matrices. In the language of a differential manifold, a 3D BZ is a three-torus T^3, while $SU(2)$ is diffeomorphic to a three-sphere S^3, and thus B_r defines a mapping $T^3 \to S^3$. For such a mapping, there exists an integer topological index, i.e., the degree $\deg[B_r]$, which measures how many times the T^3 wraps around the S^3:

$$\deg[B_r] = -\int \frac{d^3\mathbf{k}}{24\pi^2}\epsilon^{ijk}\mathrm{Tr}[(B_r\partial_i B_r^\dagger)(B_r\partial_j B_r^\dagger)(B_r\partial_k B_r^\dagger)],$$

where $\partial_i = \partial/\partial k_i$.

The definition of magnetoelectric polarization P_3 can be found in Refs. [2,10,11,31,46–49] and it is known that P_3 can be computed via the sewing matrix [10,11,47]

$$2P_3 = -\frac{1}{24\pi^2}\int d^3\mathbf{k}\epsilon^{ijk}\mathrm{Tr}[(B\partial_i B^\dagger)(B\partial_j B^\dagger)(B\partial_k B^\dagger)].$$

For a block diagonal B matrix, this integral reduces to

$$2P_3 = \sum_{r=1}^{N}\deg[B_r], \tag{2}$$

where $\deg[B_r]$ is the degree of the mapping B_r: $T^3 \to S^3$ discussed above. It is worthwhile to emphasize that only the module 2 of $2P_3$ (or $\deg[B_r]$) is gauge invariant and thus has real physical meaning. This conclusion can be easily checked by noticing that a gauge transformation can change the degree by an even integer, i.e., under $|u_n(\mathbf{k})\rangle \to |u_j(\mathbf{k})\rangle U_{jn}(\mathbf{k})$, $B(\mathbf{k}) \to U^\dagger(C_4T\mathbf{k})B(\mathbf{k})U^*(\mathbf{k})$ and $\deg[B] \to \deg[B] + 2\deg[U]$. Therefore we will only keep track of the mod 2 of the degree, which will be denoted as $\deg_2[B_r]$ in the rest of the Letter.

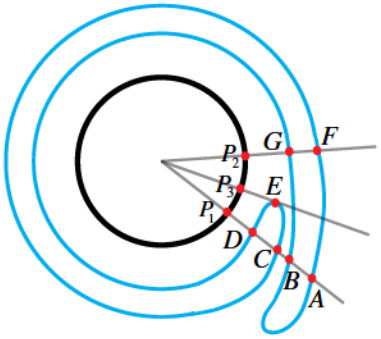

FIG. 1. Illustration of a map f: $S^1 \to S^1$ with degree 0. The black circle is the target space and the blue line demonstrates the mapping from the original space to this circle. To calculate $\deg_2[f]$, we can pick a nonsingular point like P_1 or P_2 in the target space and count the number of points that are mapped to it. There are four points mapped to P_1 and two points to P_2, therefore $\deg_2[f] = 4 \bmod 2 = 2 \bmod 2 = 0$. Note that we cannot choose P_3 to calculate the degree because the map at point E is singular.

The mod 2 of the degree can be easily calculated through a counting technique, if we realize that the degree counts how many times the original spaces wraps around the target space. Here, we first demonstrate this technique using a simple example: a mapping between 1-spheres f: $S^1 \to S^1$ shown in Fig. 1. To get $\deg_2[f]$, we take any nonsingular point in the target space and count how many points in the original space are mapped to this target point under f. If this number is n, then $\deg_2[f] = n \bmod 2$.

For B_r: $T^3 \to S^3$, it turns out that a specific gauge can be chosen, which allows the counting technique to be easily adopted. Because $C_2 = -(C_4T)^2$, C_2 is also a symmetry of the system, and therefore the $2N \times 2N$ sewing matrix $D_{mn}(\mathbf{k}) = \langle u_m(C_2\mathbf{k})|C_2|u_n(\mathbf{k})\rangle$ is unitary, where $C_2\mathbf{k} \equiv (-k_x, -k_y, k_z)$. The fact that $C_2 = -(C_4T)^2$ and $(C_2)^2 = -1$ implies [50]

$$D(\mathbf{k}) = -B(C_4T\mathbf{k})B^*(\mathbf{k}) \quad \text{and} \quad D(C_2\mathbf{k}) = -D^\dagger(\mathbf{k}). \tag{3}$$

Because C_2 does not give rise to nontrivial topology in the presence of the C_4T symmetry, there should be no topological obstruction to smoothly deform the C_2 sewing matrix $D(\mathbf{k})$ to a constant matrix independent of momentum $\mathbf{k}$. In the Supplemental Material [50] we explicitly construct a smooth gauge transformation to make $D(\mathbf{k}) = \mathrm{diag}(i\sigma_z, i\sigma_z, \ldots, i\sigma_z)$ while keeping $B_r(\mathbf{k}) \in SU(2)$. With this gauge choice, Eq. (3) implies

$$B_r(C_4T\mathbf{k}) = -i\sigma_z B_r^T(\mathbf{k}). \quad (4)$$

This condition has remarkable consequences. If $\mathbf{k}$ is a C_4T invariant point, Eq. (4) implies

$$B_r(\mathbf{K}) = \pm\frac{i}{\sqrt{2}}(\sigma_x + \sigma_y) \equiv A_\pm, \quad \mathbf{K} \in K^4, \quad (5)$$

where $K^4 = \{\Gamma, M, Z, A\}$ represents C_4T invariant points as defined early on, i.e., at C_4T invariant points, B_r can only take one of these two distinct values $A_\pm$. On the other hand, if $\mathbf{k}$ is not a C_4T invariant point and if $B_r(\mathbf{k}) = A_\pm$, then Eq. (4) implies $B_r(C_4T\mathbf{k}) = B_r(\mathbf{k}) = A_\pm$. Hence, if some $\mathbf{k} \notin K^4$ is mapped to A_+, there must be one (or three) additional momentum point (related to each other by C_4T) which is also mapped to A_+, and the same is true for A_-. Therefore if we choose A_+ (or A_-) as the special point to perform the counting described above, as far as $\deg_2[B_r]$ is concerned, only the four C_4T invariant points need to be considered, because any other point contributes even numbers to the counting. In summary, for each B_r, we only need to examine the four C_4T invariant points (K^4). If n_r of these four points are mapped to A_+ (and thus $4 - n_r$ to A_-), then $\deg_2[B_r] = n_r \bmod 2$.

Now we relate this n_r to a Pfaffian. Define

$$M_{mn}(\mathbf{k}) = \langle u_m(\mathbf{k})|\Theta|u_n(\mathbf{k})\rangle, \qquad \Theta = \frac{C_4T + C_4^{-1}T}{\sqrt{2}}, \quad (6)$$

where m, n are valence band indices. Under the gauge chosen above, at $\mathbf{K} \in K^4$, $M(\mathbf{K})$ is block diagonal $M(\mathbf{K}) = \mathrm{diag}(M_1, M_2, \ldots, M_N)$. Using the facts $(C_4)^2 = -(C_4)^{-2}$, $T^2 = -1$, and $[(C_4 + C_4^{-1})/\sqrt{2}]^2 = 1$, we show in the Supplemental Material [50] that $M(\mathbf{k})$ is antisymmetric $M^{\mathrm{T}}(\mathbf{k}) = -M(\mathbf{k})$ for every $\mathbf{k}$ in the BZ, and at C_4T invariant points $\mathbf{K} \in K^4$, $M(\mathbf{K})$ is unitary and $M(\mathbf{K}) = [B(\mathbf{K}) - B^{\mathrm{T}}(\mathbf{K})]/\sqrt{2}$. From Eq. (5), we know that for $\mathbf{K} \in K^4$, $B_r(\mathbf{K}) = A_+$ or A_- and thus, respectively, $\mathrm{Pf}[M_r(\mathbf{K})] = +1$ or -1, i.e., counting n_r is identical to counting the number of C_4T invariant momentum points with $\mathrm{Pf}[M_r(\mathbf{K})] = +1$, i.e., $(-1)^{\deg_2[B_r]} = (-1)^{n_r} = \prod_{\mathbf{K}\in K^4} \mathrm{Pf}[M_r(\mathbf{K})]$, and when contributions from all valence bands are combined, we have

$$(-1)^{2P_3} = \prod_{\mathbf{K}\in K^4} \frac{\mathrm{Pf}[M(\mathbf{K})]}{\sqrt{\det[B(\mathbf{K})]}}. \quad (7)$$

This equation is one main conclusion of this Letter. It generalizes the Pfaffian formula of Fu and Kane [4] to systems without time-reversal symmetry, via replacing the T operator with a new combination $\Theta = (C_4T + C_4^{-1}T)/\sqrt{2}$.

On the right-hand side (r.h.s.) of Eq. (7) we added by hand a denominator $\sqrt{\det B}$. In the gauge we choose above, this quantity is unity and thus does not contribute anything.

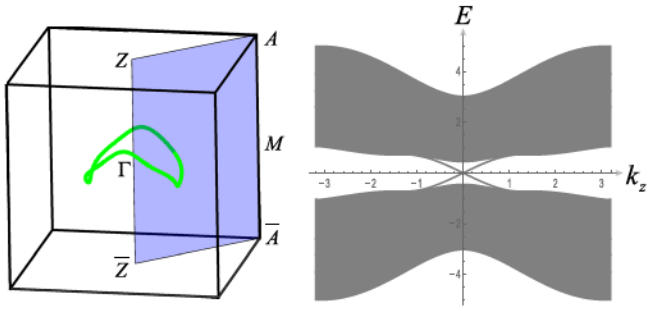

FIG. 2. Left: Schematic plot of the Brillouin zone. $\tau_{1/2}$ is the colored rectangle and $\partial\tau_{1/2}$ is its boundary. The green line represents the momenta with $\mathrm{Pf}[M(\mathbf{k})] = 0$ for the Hamiltonian shown in Eq. (16). The line of zero Pfaffian penetrates $\tau_{1/2}$, resulting in a phase winding of 2π in Eq. (15), which implies that $P_3 = 1/2$. Parameters used here are $p = 0.5$, $q_1 = 1$, $q_2 = 0.2$, $q_3 = 0.3$. Right: spectra of H as a function of k_z with open boundary condition along k_x and k_y with the same parameters. The existence of gapless hinge states suggests nontrivial topology.

However, this denominator is important, because it makes the r.h.s. gauge invariant. Thus, although our conclusion is based on a specific gauge, it remains valid regardless of gauge choices, as long as $B(\mathbf{k})$ remains smooth and a unique sign is chosen for the square root for a continuous branch of $\sqrt{\det[B(\mathbf{k})]}$, which can always be achieved because $B(\mathbf{k})$ is unitary for every $\mathbf{k}$. To demonstrate this gauge invariance, here we perform a generic gauge transformation $|u_n(\mathbf{k})\rangle \to |u_j(\mathbf{k})\rangle U_{jn}(\mathbf{k})$. Because of $\mathrm{Pf}[BAB^{\mathbf{T}}] = \mathrm{Pf}[A]\det[B]$ and $\det[BAB^{\mathbf{T}}] = \det[A]\det[B]^2$, the gauge transformation implies that $\mathrm{Pf}[M(\mathbf{K})] \to \mathrm{Pf}[M(\mathbf{K})]\det[U(\mathbf{K})]^*$ and $\sqrt{\det[B(\mathbf{K})]} \to \sqrt{\det[B(\mathbf{K})]}\det[U(\mathbf{K})]^*$. Hence the effect of the gauge transformation cancels in Eq. (7).

3D index as a 2D integral.—In this part, we will show that Eq. (7) can be expressed as a 2D integral, which greatly reduces computational cost for evaluating P_3, similar to what has been achieved in TIs [43,44]. We define another matrix for the valence bands

$$\omega_{mn}(\mathbf{k}) = \langle u_m(-\mathbf{k})|\Theta|u_n(\mathbf{k})\rangle, \quad (8)$$

with Θ defined in Eq. (6). $\omega(\mathbf{k})$ is not unitary for a generic $\mathbf{k}$, but we are mainly interested in $\omega(\mathbf{k})$ for $\mathbf{k}$ inside the straight line formed by $Z\Gamma\bar{Z}$ and $AM\bar{A}$ (Fig. 2). As shown in the Supplemental Material [50], along these two lines $\omega(\mathbf{k})$ is unitary and $\det[\omega(\mathbf{k})] = \det[B(\mathbf{k})]$. Because $\omega(\mathbf{K}) = M(\mathbf{K})$ for $\mathbf{K} \in K^4$, Eq. (7) can thus be rewritten as

$$(-1)^{2P_3} = \prod_{\mathbf{K}\in K^4} \frac{\mathrm{Pf}[\omega(\mathbf{K})]}{\sqrt{\det[\omega(\mathbf{K})]}}. \quad (9)$$

As Fu and Kane [4] have shown for TIs, Eq. (9) can also be expressed as an integral

$$2P_3 = \frac{1}{2\pi}\left[\oint_{\partial\tau_{1/2}} A d\ell - \int_{\tau_{1/2}} d\tau F\right] \mod 2. \quad (10)$$

Here $\tau_{1/2}$ refers to the rectangle $Z\bar{Z}\bar{A}A$ in Fig. 2 and $\partial\tau_{1/2}$ is its boundary. A and F are the Abelian Berry connection and Berry curvature inside $\tau_{1/2}$. If we label each wave function $|u_n(\mathbf{k})\rangle$ as $|u_r^s(\mathbf{k})\rangle$, where $r = 1, \ldots, N$ labels different Kramers pairs and $s = \mathrm{I}, \mathrm{II}$ distinguishes the two states in a Kramers pair, there is a gauge fixing condition at the boundary $Z\bar{Z}$ and $A\bar{A}$ for Eq. (10) to be valid:

$$|u_r^{\mathrm{I}}(-\mathbf{k})\rangle = \Theta|u_r^{\mathrm{II}}(\mathbf{k})\rangle, \quad (11)$$

$$|u_r^{\mathrm{II}}(-\mathbf{k})\rangle = -\Theta|u_r^{\mathrm{I}}(\mathbf{k})\rangle. \quad (12)$$

The formula here is slightly different from the one used in Ref. [4], because T is now replaced by $\Theta = (C_4T + C_4^{-1}T)/\sqrt{2}$. But for Eqs. (11) and (12), because it is evaluated only along $Z\bar{Z}$ and $A\bar{A}$, where $\Theta\mathbf{k} = T\mathbf{k} = -\mathbf{k}$, the difference between T and Θ vanishes and thus derivations in Ref. [4] can be generalized to systems studied here by simply replacing T by Θ.

Equation (10) enables us to develop efficient numerical techniques to calculate P_3 without the need for a global gauge, following a similar line of thinking as has been achieved for TIs [43,44]. The method proceeds as follows. First, let us select a discrete mesh in $\tau_{1/2}$ and define $Q_{\mu,mn}(\mathbf{k}) = \langle u_m(\mathbf{k})|u_n(\mathbf{k} + s_\mu)\rangle$, where $\mu = 1, 2$ and s_μ is the mesh step size in the two directions in $\tau_{1/2}$. Apply gauge fixing condition Eqs. (11) and (12) to the boundary $\partial\tau_{1/2}$. Let $L_\mu(\mathbf{k}) = \det[Q_\mu]/|\det[Q_\mu]|$ and $\tilde{A}_\mu(\mathbf{k}) = \ln L_\mu(\mathbf{k})$, $\tilde{F}(\mathbf{k}) = \ln[L_1(\mathbf{k})L_2(\mathbf{k} + s_1)L_1^{-1}(\mathbf{k} + s_2)L_2^{-1}(\mathbf{k})]$, where the imaginary part of all the logarithms are restricted to $(-\pi, \pi]$. Then $2P_3$ can be calculated through

$$2P_3 = \frac{1}{2i\pi}\left[\sum_{\mathbf{k}\in\partial\tau_{1/2}} \tilde{A}_\mu(\mathbf{k}) - \sum_{\mathbf{k}\in\tau_{1/2}} \tilde{F}(\mathbf{k})\right] \mod 2, \quad (13)$$

where the direction μ should be along the positive direction of $\partial\tau_{1/2}$. This numerical technique does not require a smooth gauge and is thus convenient to implement. This method has been well known for 2D and 3D TI, and is now generalized to 3D HOTI without time-reversal symmetry.

S_4 symmetry and high-symmetry points.—We show here that if the system has a fourfold rotoinversion symmetry S_4, in addition to C_4T, P_3 can be directly obtained by evaluating S_4 eigenvalues at high symmetry points. This conclusion is a generalization of the Fu-Kane's parity criterion [6] to HOTIs, with a key observation that $\tilde{S} = (S_4 + S_4^{-1})/\sqrt{2}$ and $\Theta = (C_4T + C_4^{-1}T)/\sqrt{2}$ can play the role of space inversion I and time reversal T, respectively. This correspondence can be seen from the fact that $(\tilde{S})^2 = 1$ and $\tilde{S}\Theta = IT = S_4C_4T$, which is a consequence of $(S_4)^4 = -1$ and $S_4 = IC_4^{-1}$. Then the derivations shown in Ref. [6] remain valid as long as we replace I by $\tilde{S}$ and T by Θ, leading to an expression for P_3 [50]:

$$(-1)^{2P_3} = \prod_{\mathbf{K}\in K^4}\prod_{r=1}^{N} \eta_r^{\mathrm{I}}(\mathbf{K}). \quad (14)$$

Here r runs over all occupied Kramers pairs, and K_4 is the set of S_4 invariant points and $\eta_r^{\mathrm{I}} = \pm 1$ is the eigenvalue of $\tilde{S} = (S_4 + S_4^{-1})/\sqrt{2}$. Equation (14) is a generalization of the Fu-Kane parity criterion [6] to systems with S_4 but no inversion symmetry. It is also consistent with results obtained using symmetry indicators [36,38].

Zeros of the Pfaffian.—Equation (7) also allows us to determine P_3 though the zero of $\mathrm{Pf}[M(\mathbf{k})] \equiv p_f(\mathbf{k})$. In this section, we no longer assume S_4 symmetry. Because $M(\mathbf{k})$ is antisymmetric at every momentum, its Pfaffian is a well-defined function over the whole BZ. Under a smooth gauge with $\det[B] = 1$, $p_f(\mathbf{K}) = \pm 1$ at $\mathbf{K} \in K^4$. Hence, Eq. (7) can be interpreted as the sum of phase change of $p_f(\mathbf{k})$ from Z to Γ and from M to A as shown in Fig. 2, i.e., $2P_3 = (\pi i)^{-1}\int_L d\mathbf{k}\cdot\nabla \ln p_f(\mathbf{k})$, where L is the combination of two straight paths $(Z \to \Gamma) + (M \to A)$. As proven in the Supplemental Material [50], $p_f(\mathbf{k}) = p_f(C_4T\mathbf{k})^* \det[B(\mathbf{k})]$, and thus when $\det[B] = 1$ and $\mathbf{k} \in L$, $p_f(\mathbf{k}) = p_f(-\mathbf{k})^*$. Therefore the phase change of $p_f(\mathbf{k})$ from Z to Γ is the same as that from Γ to $\bar{Z}$. With this fact we can extend the integration path L to be $\partial\tau_{1/2}$ and divide by 2 to get $2P_3$, which gives

$$2P_3 = \frac{1}{2\pi i}\oint_{\partial\tau_{1/2}} d\mathbf{k}\cdot\nabla \ln \mathrm{Pf}[M(\mathbf{k})]. \quad (15)$$

This is a generalization of the result by Kane and Mele [7], via replacing T by Θ. The r.h.s. of the equation measures the phase winding of $\mathrm{Pf}[M(\mathbf{k})]$ around the boundary of the 2D area $\tau_{1/2}$. Because a nontrivial phase winding around the 1D boundary implies nodal points in the 2D bulk with $\mathrm{Pf}[M(\mathbf{k})] = 0$, this equation implies that $2P_3$ can be obtained by counting the number of nodal points with $\mathrm{Pf}[M(\mathbf{k})] = 0$ in $\tau_{1/2}$. More details will be demonstrated below using a tight-binding model. Interestingly, here we have shown that for a 3D HOTI, its topological index P_3 can be calculated by looking at the zeros of $\mathrm{Pf}[M(\mathbf{k})]$ in a single 2D plane ($\tau_{1/2}$). This is in direct contrast to first order 3D TIs, where one needs to investigate two time reversal invariant 2D planes to determine the Z_2 index [5]. Equation (15) also implies that if $\mathrm{Pf}[M(\mathbf{k})]$ is nonzero over $\tau_{1/2}$, then P_3 will automatically be trivial.

Tight binding model.—Here we use tight-binding models to demonstrate and to verify our conclusions. Consider a four-band model with a Hamiltonian

$$H(\mathbf{k}) = (\cos k_x + \cos k_y + \cos k_z - 2)\tau_z\sigma_0 + q_1 \sum_{i=x,y,z} \sin k_i \tau_x \sigma_i + q_2 \sum_{j=x,y} \sin k_j \sin k_z \tau_y \sigma_j + q_3 \tau_x \sigma_0 + p(\cos k_x - \cos k_y)\tau_y \sigma_0. \quad (16)$$

Here $C_4 = \tau_0 e^{-i(\pi/4)\sigma_z}$, $T = -i\tau_0\sigma_y K$, $S_4 = \tau_z e^{i(\pi/4)\sigma_z}$. The Hamiltonian satisfies $C_4 T H(\mathbf{k})(C_4 T)^{-1} = H(C_4 T\mathbf{k})$. The p term breaks C_4 and T symmetry but preserves S_4 and C_4T. If p vanishes then the system becomes a 3D TI. The q_2 and q_3 terms break S_4 symmetry. When $q_2 = q_3 = 0$, S_4 symmetry is recovered and the model reduces to the one shown in Ref. [10]. In this case the Kramers pair in the valence bands at Γ has $\tilde{S}$ eigenvalue -1 and all other S_4 invariant points have $\tilde{S}$ eigenvalue $+1$. Thus by Eq. (14), we have $P_3 = 1/2$ and the system is a CSOTI. When small q_2 and q_3 are turned on, the band gap does not close and the system should still remain a CSOTI. We calculate the zero of $\mathrm{Pf}[M(\mathbf{k})]$ as shown in Fig. 2. The zeros form a loop penetrating $\tau_{1/2}$, giving rise to a phase winding of 2π in $\mathrm{Pf}[M(\mathbf{k})]$. Therefore, from Eq. (15), $P_3 = 1/2$. We also apply Eq. (13) and get $P_3 = 1/2$ as well. To verify our prediction we diagonalize the system with open boundary condition along k_x and k_y, and the spectra as a function of k_z is shown in Fig. 2. Gapless hinge states are found, which confirms that the system is a CSOTI with $P_3 = 1/2$.

Conclusions and discussions.—In this Letter, we generalize the Pfaffian topological invariant to higher-order topological insulators, utilizing a composite operator composed of linear superposition of symmetry operators. In addition to the C_4T-invariant systems discussed above, this construction applies generically to systems with symmetry-enforced Kramers-like degeneracy (see S-6 in the Supplemental Material [50] for more details). In addition, this Pfaffian formula is directly related with the dipole pumping and the nontrivial Wannier-band Chern numbers [8,9], as shown in S-7 in the Supplemental Material [50]).

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