Universal higher-order bulk-boundary correspondence of triple nodal points

Patrick M. Lenggenhager 1,2,3,* Xiaoxiong Liu 3, Titus Neupert 3, and Tomáš Bzdušek 1,3,†

1Condensed Matter Theory Group, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland
2Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland
3Department of Physics, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland

*Corresponding author: lenpatri@ethz.ch
†Corresponding author: tomas.bzdusek@psi.ch

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Triple nodal points are degeneracies of energy bands in momentum space at which three Hamiltonian eigenstates coalesce at a single eigenenergy. For spinless particles, the stability of a triple nodal point requires two ingredients: rotational symmetry of order three, four, or six; combined with mirror or space-time-inversion symmetry. However, despite ample studies of their classification, robust boundary signatures of triple nodal points have until now remained elusive. In this work, we first show that pairs of triple nodal points in semimetals and metals can be characterized by Stiefel-Whitney and Euler monopole invariants, of which the first one is known to facilitate higher-order topology. Motivated by this observation, we then combine symmetry indicators for corner charges and for the Stiefel-Whitney invariant in two dimensions with the classification of triple nodal points for spinless systems in three dimensions. The result is a complete higher-order bulk-boundary correspondence, where pairs of triple nodal points are characterized by fractional jumps of the hinge charge. We present minimal models of the various species of triple nodal points carrying higher-order topology, and illustrate the derived correspondence on Sc2AlC which becomes a higher-order triple-point metal in applied strain. The generalization to spinful systems, in particular to the WC-type triple-point material class, is briefly outlined.

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I. INTRODUCTION

The hallmark feature of higher-order topological phases in \( d \) dimensions is the presence of an anomaly on boundaries with dimensions \( d - 2 \) or lower [1–23]. In two dimensions (2D), second-order crystalline topological insulators require additional chiral symmetry or particle-hole symmetry to protect zero-energy corner modes [11,24–26]. If such symmetries are absent and the corner modes merge into the bulk energy bands, the nontrivial second-order topology is instead revealed by a corner-induced filling anomaly [3,27–29], i.e., an obstruction to simultaneously satisfying charge neutrality and preserving the crystalline symmetries in the presence of corners. In particular, if the valence bands are filled and the crystalline symmetry preserved, the filling anomaly implies corner-localized charges. Remarkably, in the presence of rotational symmetry, the corner charges acquire fractional quantized values that can be predicted [28,30,31] using symmetry indicators [32–39], i.e., symmetry eigenvalues of the occupied bands at high-symmetry points (HSPs) in the Brillouin zone (BZ).

The notion of higher-order topology has recently been generalized to three-dimensional (3D) nodal phases with twofold and fourfold degeneracies, resulting in higher-order Weyl [40–44] and Dirac [9,45–47] semimetals, respectively, as well as to a class of nodal-ring semimetals obtained by perturbing Dirac degeneracies [48]. Such semimetals can be understood as 2D topological insulators which are augmented by a third dimension along which the higher-order topology changes, with the band nodes marking the occurrence of higher-order phase transitions. Correspondingly, higher-order topological semimetals are characterized by zero-energy hinge states (in the presence of chiral symmetry) or fractional hinge charges (in their absence) for a range of momenta demarcated by the band degeneracies. In light of these observations, a question of timely interest arises, namely, whether the phenomena associated with higher-order topology also extend to more intricate species of band nodes.

Triple nodal points [49–58] [triple points (TPs) for short] are threefold degeneracies of energy bands occurring at points in momentum space, and therefore constitute intermediates between Weyl and Dirac points. They occur on high-symmetry lines (HSL) in the BZ when a twofold-degenerate band [corresponding to a 2D irreducible corepresentation (ICR) of the HSL’s little cogroup and forming what we call the central nodal line (NL)] is crossed by a third nondegenerate band [one-dimensional (1D) ICR of the little cogroup] [51]. In some cases, TPs are accompanied by additional NL arcs that lie off the rotation axis but coalesce with the central NL at a nexus point [59]. Triple points are thus classified [49,58–60] as type B if a nexus point coincides with the TP and as type A otherwise (where the appearance of a nexus point near the TP is optional). TPs were shown by angle-resolved photoemission spectroscopy to exist in the band structure of MoP [53] and WC [54].

In contrast to Weyl and Dirac points, a single TP generically results in a metallic state, due to the imbalance between the degeneracy of the crossing bands. However, pairs of TPs,
formed when the 2D ICR consecutively crosses two 1D ICRs, can result in a semimetal with small Fermi pockets. We call such a TP configuration a triple-point pair (TPP). These nodal features can arise both in spinful [49] and spinless [51,60] systems; however, although there have recently been several efforts [59–63] towards their topological description and symmetry classification, it has remained an open question whether TPs or TPPs can be characterized by robust boundary signatures.

In this work, we answer both postulated questions in a single stroke: semimetallic TPPs are generally characterized by a higher-order bulk-boundary correspondence; namely, each species of TPP can be assigned a unique value of fractional jump of the hinge charge. We derive the exact correspondence by combining the symmetry classification of TPs [59,60] with the symmetry indicators of higher-order topology. Note that while we explicitly consider only TPs occurring in spinless systems, our mathematical analysis based on symmetry indicators can be easily generalized to the spinful case [59,60].

The diverse range of symmetry combinations seemingly complicates the analysis. However, it turns out that all the cases of interest can be obtained by a proper perturbation of a system with \( PT \) symmetry. Therefore, our approach to analyze the topological invariants and the bulk-hinge correspondence of TPPs is to first deal with the \( PT \)-symmetric cases, and afterwards consider the effect of perturbations to derive the results also for the \( PT \)-broken cases. In particular, in the presence of \( PT \) we can characterize the TPP also by a second Stiefel-Whitney (2SW) or Euler monopole charge, of which the first one provides further insights into the bulk-hinge correspondence [19,22]. Our results for the correspondence between TPs, and their associated fractional jump in the hinge charge, and (if also defined) their 2SW and Euler monopole charges, are summarized in Table II. The results also apply to nonsymmorphic space groups (SGs) with appropriate identification of ICRs [59].

The paper is organized as follows. In Sec. II, we present a concrete \( C_4 \)-symmetric tight-binding model that illustrates the phenomenology of TPP-induced higher-order topology,
including both the hinge-charge jump and the 2SW monopole invariant. This motivates our study and sets the stage for the subsequent general discussion. First, Sec. III discusses monopole charges induced by type-A TPs in PT-symmetric spinless systems using simple manipulations with the non-Abelian band topology. The analysis reveals that pairs of TPs in three-band models can be characterized by the Euler monopole charge, while TPs in four-band models can carry the 2SW monopole charge. The discussion is then substantially generalized in Sec. IV, where we use symmetry indicators to establish the main result of our work: a general bulk-hinge correspondence principle for TPs in spinless systems. As intermediate results, we are led to also derive symmetry-indicator formulas for the 2SW and Euler monopole charge in the presence of rotational symmetry and a bulk-corner correspondence principle for the former, and we analyze the effect of symmetry breaking on TPs. For simplicity, we first focus on symmorphic SGs and discuss the generalization to nonsymmorphic SGs only in Sec. VII.

After presenting the main results of our theoretical analysis, we apply the theory to concrete models. First, in Sec. V, we demonstrate the derived bulk-hinge correspondence on minimal tight-binding models for various TPs species. We first revisit the C4v-symmetric model from Sec. II and then discuss concrete Hamiltonians for the C6v- and C3-symmetric cases. Next, we consider two material examples in Sec. VI. On the one hand, we consider Sc2AlC in large uniaxial strain to provide a solid-state illustration of TPs with the predicted fractional hinge-charge jump. On the other hand, we show that Li2NaN under ambient conditions has a pair of TPs carrying a nontrivial Euler monopole charge, and we briefly discuss the consequences of this topological obstruction on the stability of the band nodes. In Sec. VII, we first explain how the symmetry-indicator formulas for the corner charge can be applied to compute the fractional hinge charge in a wire geometry even for nonsymmorphic SGs and then argue that the bulk-hinge correspondence of TPs generalizes to nonsymmorphic SGs. Then, in Sec. VIII we present a short digression to TPs in spinful systems, and argue that strongly spin-orbit-coupled compounds in the WC-type crystal structure studied by Ref. [49] could host the fractional hinge-charge jumps. Finally, we conclude in Sec. IX by summarizing the main results and outlining possible extensions of our work to other nodal configurations.

The main text is accompanied by several Appendixes which discuss details of our theoretical and numerical analysis: In Appendixes A and B we summarize our mathematical derivations that involve the symmetry indicators, in Appendix C we include details of the presented tight-binding models and explain how they were systematically constructed, in Appendix D we present methods to numerically extract the hinge charges from tight-binding models. Finally, in Appendix E we discuss the Euler monopole charge from the perspective of the non-Abelian band topology (significantly extended in the Supplemental Material [72], where we prove a conjecture relating the non-Abelian invariant computed on contours shifted by reciprocal lattice vectors) and illustrate this on several material examples.

II. HINGE CHARGES INDUCED BY TRIPLE POINTS

To motivate our study of higher-order topology associated with TPs, we introduce a concrete model and investigate its phenomenology. The model assumes spinless particles on a tetragonal lattice (with lattice constants set to $a = c = 1$ for simplicity) and has the (symmorphic) SG P4/mmm (No. 123) with isogonal point group $D_{4h}$. As illustrated in Fig. 1(a), we place $(p_x, p_y)$ orbitals transforming in the ICR $E_u$ at Wyckoff position (WP) 1a, and the orbitals $d_{xy}$ and $d_{x^2-y^2}$, transforming in $B_{1g}$ and $B_{2g}$, respectively, at WP 1c. The site-symmetry group of both considered WPs corresponds to the complete $D_{4h}$ point group.

In the basis $(|p_x, ip_y, dp_{xy}, dp_{x^2-y^2}\rangle$, the considered model is expressed by the Bloch Hamiltonian

$$H(k) = \begin{pmatrix} -t_1+2t_2(\cos k_x+\cos k_y+\cos k_z) & \gamma_3 & t_3(\gamma_{14} - \gamma_{25}) \\ -t_4(\cos k_x-\cos k_y)(\gamma_{14} + \gamma_{25}) & \gamma_4 & \gamma_5 \\ 2t_5 \sin k_x \sin k_y(\gamma_{13} - \gamma_{24}) & -2t_6(\cos k_x + \gamma_3) & \gamma_6 \end{pmatrix},$$

where $t_1, t_2, t_3, t_4, t_5, t_6$ are the hopping parameters.

FIG. 1. Features of the model given in Eq. (1). (a) Real-space unit cell spanned by the lattice vectors $a_{1,2,3}$ with the four orbitals: $(p_x, p_y)$ at Wyckoff position 1a and $d_{xy}$, $d_{x^2-y^2}$ at 1c. (b) Single layer (for fixed $z$) of the three-dimensional lattice. The blue shaded regions indicate the projection of the unit cells with the orbitals indicated in the same colors as in (a). Black lines (where further symmetry-related lines are dropped to maintain clarity) indicate the in-plane hopping processes included in the model. (c) Band structure along the high-symmetry lines. (d) Brillouin zone spanned by the reciprocal lattice vectors $G_{1,2,3}$ with high-symmetry points $\Gamma, Z, X, R, M, A$ shown. Nodal lines in the first, second, and third band gaps are displayed in orange, red, and blue color, respectively. The four triple points of the model are indicated by green arrows in (c) and (d).
where $\gamma_1 = \sigma_x \otimes \tau_z$, $\gamma_2 = \sigma_x \otimes \tau_x$, $\gamma_3 = \sigma_i \otimes \tau_z$, $\gamma_4 = \sigma_i \otimes \tau_x$, and $\gamma_5 = \sigma_i \otimes 1_z$, are gamma matrices obeying $\{\gamma_\alpha, \gamma_\beta\} = 2\delta_{\alpha\beta}$, and $\gamma_{ab} = \frac{1}{2} [\gamma_\alpha, \gamma_\beta]$; Pauli matrices $\sigma_i$ act on the WP degree of freedom, and Pauli matrices $\tau_j$ act on the orbital degree of freedom at fixed WP. The point group is generated by a $\frac{\pi}{2}$ rotation around the $z$ axis $C_4 = -\text{diag}(i\tau_z, 1_z)$, a $\pi$ rotation around the $y$ axis $C_2 = -\sigma_i \otimes \tau_z$, and inversion $\mathcal{I} = -\sigma_i \otimes 1_z$. Additionally, the Hamiltonian possesses time-reversal symmetry $T$. Note that we have intentionally chosen the basis of $p$ orbitals to be imaginary, which results in $\mathcal{PT} = \mathcal{K}$, such that the Bloch Hamiltonian is a real matrix [73]. In real space, Eq. (1) corresponds to the tight-binding model with charge (2 metrics of the Hamiltonian. Furthermore, we choose the ionic is displayed in Fig. 2(a) and is chosen to respect all the sym-
flakes as shown in (a) that are characterized by a corner charge $Q_k$. The edge charge of the model vanishes. For reference, the bulk band structure along $k_z$ for $k_x = k_y = 0$ is displayed in gray with the 1D (2D) degenerate bands plotted by a thin (thick) line. (c), (d) Wilson-loop spectrum of the two occupied bands in the 2D BZ for fixed $k_z = 0$ and $\pi$, respectively. For $k_z = 0$ (c) we observe a winding with odd parity, indicating a nontrivial 2SW class.

![Fig. 2](image-url)

To uncover signatures of higher-order topology, we now consider a nanowire geometry, i.e., a system which is finite in $x$ and $y$ but infinite in $z$ direction, at half-filling. Thus, only the momentum $k = [k_x, k_y, 0]$ that runs along the fourfold rotation axis remains a good quantum number and the BZ is reduced to a hinge Brillouin zone. The considered in-plane termination is displayed in Fig. 2(a) and is chosen to respect all the sym-
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the relation between monopole charges and multiband nodal links. These insights will readily explain the 2SW class observed in this section’s model. In Sec. IV, we then adopt the method of symmetry indicators and generalize the observations discussed above to establish a comprehensive bulk-hinge correspondence for TPPs. Finally, in Sec. V we first revisit this section’s model in the light of those general results, before discussing two \( C_6 \)-symmetric examples: one with type-A TPs and one with type-B TPs.

### III. MONOPOLE CHARGES INDUCED BY TRIPLE POINTS

In this section we argue that pairs of type-A TPs in spinless systems can be imbued with monopole charges. This conclusion is achieved by adopting the geometric interpretation of monopole charges as linking numbers \([70,71]\). After presenting the general argument, we apply it to two specific configurations of type-A TPs: a four-band configuration resulting in a nontrivial second Stiefel-Whitney (2SW) monopole charge in Sec. III A, and a three-band configuration resulting in a nontrivial Euler (but trivial 2SW) monopole charge in Sec. III B. In both cases we elaborate on the implications of the monopole charge on the stability of the NL segments and on the bulk topology. (NL segments demarcated by type-B TPs are not easily analyzed through the geometric method considered in the present section. We address them using the more general framework of symmetry indicators in Sec. IV.)

The 2SW class \( w_2 \) is a stable \( \mathbb{Z}_2 \)-valued invariant defined on a closed 2D manifold with a spectral gap whenever there is an antiunitary momentum-preserving symmetry squaring to \(+1\), such as \( PPT \) or \( C_2 \) \([19]\). Note that we require only one gap, here the principal gap, to be open on the 3D manifold. The 2SW class remains well defined in the presence of nodes in other band gaps. On a spherical surface enclosing nodal-ring degeneracies in 3D, the 2SW class defines a monopole charge that enhances the stability of the node \([67,68,70]\). For 2D insulating systems, on the other hand, the 2SW class on the BZ torus defines a bulk topological invariant of the full system \([19,20,22,70]\) similar to the Chern number.

The \( \mathbb{Z} \)-valued fragile extension of the 2SW class, which can be defined for a two-band subspace separated from the rest of the spectrum by energy gaps, is the Euler class \( \chi \) \([68,74,75]\). Note that only its absolute value is gauge invariant \([73]\) (see also Appendix B 3); we will therefore restrict \( \chi \) to non-negative values. Under the addition of trivial bands to the two-band subspace, only the parity of the Euler class is stable and reduces to the 2SW monopole charge discussed above, \( w_2 = \chi \mod 2 \).

We now investigate the monopole charges associated with configurations of TPs. For concreteness, in this section we focus on NL segments that are demarcated by a pair of type-A TPs (this, in particular, implies the presence of \( C_6 \) symmetry with \( n = 4 \) or \( 6 \) \([60]\)). We will call the energy gap in which that NL segment is formed the principal gap \([73]\). To understand why such NL segments could carry a nontrivial monopole charge, consider one such NL segment and require that there are no additional band nodes in the principal gap for the considered range of \( k_z \). Two examples of such configurations are shown in Figs. 3(b) and 5(a), where nodes in the principal gap are shown in red.

As has been argued in Ref. \([60]\), adding a small \( C_6 \)-breaking but \( PPT \)-preserving perturbation transforms TPs into multiband nodal links as illustrated in Figs. 3(c) and 5(b) and 5(c). Crucially, the linked nodal rings are in band gaps adjacent to each other, and such linking was shown to be in a one-to-one correspondence \([70,71]\) with monopole charges. Thus, there potentially is a nontrivial monopole charge on a surface enclosing the nodal ring of interest [purple ellipsoid in Figs. 3(c) and 5(b) and 5(c)]. By continuity we can switch this perturbation off without closing the principal energy gap on the enclosing surface, which allows us to assign the same monopole charge also to the original NL segment, i.e., on the ellipsoid in Figs. 3(b) and 5(a). In the following two subsections we investigate in detail the implications of the linking for the bulk topology of the two specified type-A TP configurations.

#### A. Second Stiefel-Whitney monopole charge from triple points

We first analyze the four-band configuration with two TPs, in which case the 2D ICR is transferred from occupied to the unoccupied bands along a rotation axis (without loss of generality set to \( k_z \)) as shown in Fig. 3(b), similar to the case of the model discussed in Sec. II. We call such a configuration of TPs a triple-point pair (TPP). It involves three species of NLs, displayed in the figures in orange, red, and blue according to increasing band index. The individual TPs correspond to locations where the 2D ICR transfers from one energy gap to another. Due to the periodicity in \( k_z \), the minimal model of such a configuration involves two such TPPs [cf. Fig. 3(a)].
Here it is sufficient to consider the upper half of the BZ. Fig. 3(b), with one (red) NL segment in the principal gap. Applying the argument outlined above for the purple ellipsoid shown in the figure, we consider a small perturbation leading to the multiband nodal link [60] [cf. Fig. 3(c)]. Since one NL in each of the two adjacent band gaps (first and third) is linked with the red nodal ring, the purple ellipsoid carries nontrivial 2SW monopole charge \( w_2 = 1 \) [70]. This has immediate consequences for the stability of the red NL segment and thus for the two TPs in Fig. 3(b). In particular, the monopole charge guarantees the persistence of the red NL even when the rotational symmetry is broken (and the 2D ICR split) as long as the \( PT \) symmetry is preserved.

We next discuss implications of the monopole charge for the bulk topology. Assuming there are no additional NLs in the principal gap in the relevant \( k_z \) range, the ellipsoid enclosing the red NL segment can be continuously deformed as illustrated in Fig. 4(a) until it spans the whole BZ in \( k_x \) and \( k_y \) directions for a finite range of \( k_z \). Due to the periodicity in the BZ, the contributions from opposite vertical faces of that surface cancel and we are left with the two horizontal planes \( T_1 \) and \( T_2 \) shown in Fig. 4(b). Note that these are actually 2D tori which can be interpreted as the BZs of certain 2D systems, namely, ones with the two-dimensional Hamiltonians \( \mathcal{H}_0(k_x, k_y) := \mathcal{H}(k_x, k_y, k_z) \).

Owing to the continuous deformation of the surface, the 2SW class does not change, such that \( \omega_2(T_1) + \omega_2(T_2) = 1 \) mod 2. Consequently, one of the two planes will be trivial, \( \omega_2 = 0 \), and the other nontrivial, \( \omega_2 = 1 \). Viewing them as 2D systems as described above, the latter is a 2D insulator with nontrivial 2SW class, called Stiefel-Whitney insulator (SWI) [70]. In the simultaneous presence of \( C_2 \) rotational and of chiral symmetry, SWIs were shown [19,22] to have robust zero-energy corner states accompanied by half-integer corner charges. Our situation is different: we do not assume chiral symmetry, and the order of rotational symmetry necessary to protect type-A TPs is \( n \in \{4, 6\} \). Until now, the (higher-order) bulk-boundary correspondence for (nonchiral) SWIs with rotational symmetry has not been clarified. We derive this piece of information in Sec. IV A; in particular, we show that the corner charge in the presence of trivial (nontrivial) 2SW class is quantized to even (odd) multiples of \( \frac{\pi}{2} \). We subsequently apply the result to study the bulk-hinge correspondence for TPs of both type A and type B in Sec. IV C.

**B. Euler monopole charge from triple points**

An even simpler configuration is obtained in a three-band model with two type-A TPs formed by the same triplet of energy bands, as illustrated in Fig. 5(a). Since the ordering of the ICRs along the rotation \( (k_z) \) axis has to be the same at both \( k_z = -\pi \) and \( \pi \) due to the periodicity of the momentum space, it again follows that the number of TPs formed by the three bands is even. In the minimal model, the NL changes the band gap twice, once from the second (blue) to the first (red) and once back to the second gap, at two TPs (yellow dots). Here we assume a single occupied and two unoccupied bands, such that the two-band subspace allows us to define the Euler monopole charge \( \chi \in \mathbb{Z} \) on the purple ellipsoid in Fig. 5(a) [68].

The Euler monopole charge of a nodal ring is determined by the linking with NLs in the adjacent band gap, similar to the case of the 2SW class, such that we can again apply the argument with the breaking of the rotational symmetry. However, here the orientation of the linked NLs becomes important [71]. Recall that in a generic multiband setting the orientation of a NL can be formally defined via the non-Abelian generalized quaternion invariant [66]. In particular, this orientation obeys the same noncommutative rules as the winding number of point nodes in 2D as reported by Ref. [19], allowing us to interpret the NLs as braid trajectories. The orientation [indicated by arrows in Figs. 5(b) and 5(c)] of the adjacent (blue) NL at the point where it crosses the disk bounded by the principal (red) nodal ring determines the flux \( \pm 1 \), indicated in gray. We observe that two distinct scenarios can arise after breaking the rotational symmetry: Fig. 5(b) where the total flux vanishes, and Fig. 5(c) where it is nonvanishing. According to Ref. [71] the former implies \( \chi = 0 \) and the latter \( |\chi| = 2 \).

While we have so far only established the possibility of the red NL segment carrying a nontrivial Euler monopole charge, the two cases \( \chi = 0 \) and \( |\chi| = 2 \) can be distinguished based on the Zak-Berry phases \( \phi_{2,3} \in [0, \pi] \) along the \( k_z \) axis of the two bands involved in the formation of the blue NL in the adjacent energy gap, i.e., the NL segment on the opposite side of the triple point than the segment under consideration. Assuming the minimal model with only a single pair of TPs along \( k_z \), as shown in Fig. 5, there are in fact only two nodal rings (the red one in the center, and the blue one on the boundary), since the two blue NL segments belong to the same nodal ring, only shifted by a reciprocal lattice vector \( \mathbf{b} \). Notably, the two copies of the blue NL ring do not necessarily exhibit consistent orientations: the orientation of a NL...
between bands 2 and 3 at \( \mathbf{k} + \mathbf{b} \) is reversed compared to the one at \( \mathbf{k} \) if and only if \( \phi_2 + \phi_3 = \pi \mod 2\pi \). In Appendix E (with additional information detailed in the Supplemental Material [72]), we formalize this statement in the framework of the non-Abelian generalized quaternion invariant [66, 71]. The result applies to an arbitrary number of bands and provides a general transformation rule for the NL orientation between neighboring BZs depending on the Berry phases.

The orientation reversal can be related to the properties of Dirac points in 2D derived in Ref. [19] if we consider a 2D cut [brown plane in Fig. 6(a)] through the BZ that intersects the blue NLS. Note that continuity implies that the two upper point nodes [i.e., upper two blue dots in Fig. 6(b)] have opposite winding number because they correspond to cuts through the same nodal ring, i.e., they manifestly annihilate when sliding the plane away from the nodal-link composition. According to Ref. [19] the copy of the uppermost node with winding number +1 in an adjacent BZ (bottom-most node), i.e., shifted by the reciprocal lattice vector \( \mathbf{b} \), has winding number \((-1)_s\), where \( s = e^{i(\phi_2 + \phi_3)} \) and \( \phi_j \) is the Zak-Berry phase of band \( j \) on the contour \( \gamma \) winding around the 2D BZ in the direction of \( \mathbf{b} \).

Although the even-valued Euler class is a fragile topological invariant, it may still imply unusual stability of the corresponding NL under perturbations, which we briefly investigate in Sec. VI B. The following Secs. IV and V investigate in more detail the case of TPs in the four-band configuration, which may exhibit the stable 2SW class, and we derive their associated signatures in the fractional hinge charges.

**IV. HIGHER-ORDER BULK-BOUNDARY CORRESPONDENCE**

In this section we mathematically establish the higher-order bulk-boundary correspondence principle foreshadowed in Sec. II: a triple-point pair (TPP) in a SG with (antiunitary) rotational symmetry of order \( n \in \{2, 3, 4, 6\} \) is generally associated with a fractional jump of the hinge charge. While the previous Secs. II and III explicitly considered only type-A TPs in systems with \( \mathcal{PT} \) symmetry, the discussion in this section is more general and encompasses all the TPs reported by the classification in Refs. [59, 60] and reproduced in Table I in symmorphic SGs. (We discuss the generalization to nonsymmorphic SGs in Sec. VII.) Furthermore, we report a correspondence between the 2SW monopole charge (if it is defined) of the NL segment connecting the two TPs and the value of the hinge-charge jump: a trivial 2SW monopole charge implies a \( \pm \frac{\pi}{n} \) jump, while a nontrivial value results in a jump by \( \pm \frac{2\pi}{n} \). We remark that the hinge-charge jump associated with a TPP always occurs without a change in the bulk polarization. This implies that if there is no fractional surface charge appearing on one side of the TPP, then there is also no fractional surface charge on the other side of the TPP, thus guaranteeing that the fractional jump in the hinge charge is observable.

We begin in Sec. IV A by discussing the 2D SWI with \( C_n \)-rotational symmetry. Here, we adapt the \( C_n \)-symmetry-indicator formula [19] for the 2SW class to \( C_n \)-rotational symmetry, where \( n \in \{4, 6\} \), and show that the value of the
2SW class constrains the possible fractional corner charges of the $C_n$-symmetric 2D system with vanishing bulk polarization. Subsequently, by temporarily adopting a stronger assumption on energy gaps in the band structure, we derive in Sec. IV B a symmetry-indicator formula for the Euler monopole charge of TPPs in the presence of $C_4$ rotational symmetry. In Sec. IV C, we combine the results obtained in the previous two subsections with the classification of TPPs to derive the general bulk-hinge correspondence principle for all possible TPP configurations in $\mathcal{PT}$-symmetric systems. Finally, in Sec. IV D, we discuss the effect of breaking various symmetries; in particular, we extend the bulk-hinge correspondence principle to TPPs protected by all MPGIs listed in Table I. Our results for the bulk-hinge correspondence are compactly summarized in Table II, while Table III compiles the various topological phase transitions induced by symmetry breaking.

A. Stiefel-Whitney insulator with rotational symmetry

We consider an insulating 2D system with $C_2T$ and $C_n$ symmetry, where $C_2$ and $C_n$ are with respect to the same axis perpendicular to the system. Due to the $C_2T$ symmetry (where $C_2$ acts like inversion in 2D) the insulator is characterized by the 2SW class, while the $C_n$ symmetry implies fractional corner charges [28–30] if the edge charge vanishes. For simplicity we assume that all the positive ionic charge, which compensates for the negative charge of the filled electron bands, is located at the maximal Wyckoff position 1a, i.e., the center of the square unit cell. In Sec. IV C we will see that for $n = 3$, the 2SW class is not symmetry indicated. Thus, we restrict the present discussion to $n = 4, 6$, which implies that $C_2$ and $T$ symmetry are also symmetries of the system.

In the following we use symmetry indicators to derive constraints on the corner charges due to a nontrivial 2SW class. We adopt the notation of Ref. [28], where the eigenvalues of the $C_n$-rotation operator at the $C_n$-symmetric HSP $\Pi$ for spinless particles are denoted by

$$\Pi^{(p)} = e^{2\pi i (p - 1)/n}, \quad p = 1, 2, \ldots, n$$

(2)

and define the quantities

$$\Pi^{(p)} = \#\Pi^{(p)} - \#\Pi^{(p)},$$

(3)

where $\#\Pi^{(p)}$ and $\#\Pi^{(p)}$ are the number of occupied energy bands with eigenvalue $\Pi^{(p)}$ at HSPs $\Pi$ and $\Gamma$, respectively. For $C_4$ we have HSPs $\Gamma, X,$ and $M,$ while for $C_6$ they are $\Gamma, M,$ and $K$. Then, assuming the specific geometries of the 2D crystals shown in Fig. 7(a), the corner charges are given by [30]

$$Q_{(4)} = \frac{e}{4} \left( \frac{1}{2} + 2\mathbb{M}^{(4)} + 3\mathbb{M}^{(4)} \right) \mod e,$$  

(4a)

$$Q_{(6)} = \frac{e}{6} \left( \mathbb{M}^{(6)} + \frac{3}{2}\mathbb{K}^{(1)} \right) \mod e,$$  

(4b)

where $e < 0$ is the electron charge and $\mod e$ implies that the center of the $C_4$-symmetric crystal is located at Wyckoff position 1a (upper sign) or 1b (lower sign). Note that, consistent with the assumptions in the present discussion, Eq. (4) assumes the presence of time-reversal symmetry $T$ with $T^2 = +1$; if $T$ is not a symmetry, Eqs. (4a) and (4b) should be used instead.

Since both $C_4$ and $C_6$ symmetries imply the presence of $C_2$ symmetry, we can also consider the symmetry-indicator formula for the 2SW class [70], namely,

$$w_2 = \sum_{\Pi \in \mathrm{TRIM}} \left( \frac{1}{2} \#\Pi^{(2)} \right) \mod 2,$$  

(5)

where the sum is over the four time-reversal-invariant momenta (TRIM) in the BZ (these are exactly the $C_2$-invariant momenta) and $\lfloor \cdot \rfloor$ is the floor function. In Appendix A 2 we show that in the presence of an enlarged rotational symmetry, the 2SW class can be equivalently written as

$$C_4 : \quad w_2 = \frac{1}{2} \mathbb{M}^{(4)} \mod 2,$$  

(6a)

$$C_6 : \quad w_2 = \frac{1}{3} \mathbb{M}^{(6)} \mod 2,$$  

(6b)

where on the right-hand side we used the same $C_n$ symmetry indicators that also enter Eq. (4).

Finally, we observe that for vanishing polarization, the 2SW class constrains the corner charge. For $n = 4$ the polarization vanishes if and only if $|X^{(2)}_{1}| = 0 \mod 2$, while for $n = 6$ it always vanishes [28]. Therefore, vanishing polarization also implies that the center-dependent sign ambiguity in Eq. (4a) drops from our analysis. Combining the assumption of vanishing polarization with Eqs. (4) and (6), we show in Appendix A 2 that the nontrivial value $w_2 = 1$ constrains the corner charge for $C_4$-symmetric SWIs to

$$Q_{(4)}^{(4)} \in \left\{ \pm \frac{e}{4} \right\} \mod e,$$  

(7a)

and for $C_6$-symmetric SWIs to

$$Q_{(6)}^{(6)} \in \left\{ \pm \frac{e}{6}, \frac{e}{2} \right\} \mod e,$$  

(7b)

i.e., to odd multiples of $\frac{e}{6}$, whereas the complementary fractional values correspond to insulators with $w_2 = 0$.

Before applying the presented formulas to study TPPs in 3D, we briefly comment on some relations of the result in Eq. (7) to previous works. First, note that in the presence of chiral symmetry, the corner charge can only attain value 0 or $\frac{e}{2} \mod e$. This can be easily understood as follows. If the occupied states carry localized corner charge $Q$ $\mod e$, then (by completeness of the Hilbert space) the unoccupied states carry localized corner charge $-Q$ $\mod e$. Chiral symmetry is local in real space and maps occupied onto unoccupied states, therefore guaranteeing that $Q = -Q$ $\mod e$.

FIG. 7. (a) The $C_4$-symmetric cross-section geometries for which the hinge charges are defined, and for which the values listed in Table II apply. The corners (gray regions) in the cross sections correspond to the hinges in the 3D system. (b) Deformation of the $C_6$-symmetric sample (inner hexagon) to a $C_4$-symmetric sample (outer triangle). Two corners (blue and green) of the hexagon with corner charges $Q^e$ and $Q^o$ merge into a single corner (red) of the triangle with corner charge $Q^{e+o} = Q^e + Q^o$. 
That equation has two solutions: $Q = 0$, $\frac{\pi}{2} \mod e$. On the other hand, our derivation in Appendix A2 reveals that the value $w_2 = 1$ can result in corner charge $Q^{(6)} = \frac{\pi}{2} \mod e$ if and only if $[K^{(3)}_4] = 0 \mod 6$. This is compatible with the finding of Ref. [76] which showed that chiral symmetry that commutes with $C_4$ rotation implies $[K^{(3)}_4] = 0$. The value $\frac{\pi}{2} \mod e$ of the corner charge was also reported in the study of a SWI model with chiral and $C_4$ symmetry by Ref. [19]. Second, the result in Eq. (7a) implies that the three conditions (1) $C_4$ symmetry, (2) $w_2 = 1$, and (3) vanishing polarization are incompatible with (4) the presence of chiral symmetry; equivalently, SWI with chiral and $C_4$ symmetries must necessarily have gapless edges. This finding is compatible with the observations of Ref. [48] made in the context of second-order NL semimetals.

### B. Euler monopole charge in presence of rotational symmetry

If the two occupied bands involved in the TPP formation are separated from lower-lying occupied bands by an energy gap, the 2SW can be refined to the Euler monopole charge. Note that this is a different situation from the one discussed in Sec. III B: here we consider a surface enclosing a TPP, i.e., two TP in adjacent band gaps, as shown in Fig. 3(b). Monopole charges such as the 2SW and the Euler monopole charge can be inferred from the winding of the Wilson-loop spectrum. Symmetries constrain the latter [33,77,78] and therefore lead to symmetry-indicator formulas for the monopole charges. To our knowledge, no such symmetry-indicator formulas for the Euler monopole charge in the presence of rotational symmetry have been previously derived, therefore, we do that here.

Along the way, we identify that TP$s$ formed by certain combinations of ICRs are necessarily associated with extended NLs in the principal gap, which prevents the system from exhibiting higher-order topological signatures and the monopole charge from being defined. The details of these derivations are relegated to Appendix B, while here we only outline the main steps and results.

To derive the symmetry-indicator formulas, we consider a spherical surface enclosing part of a HSL with $C_n$ rotational symmetry in its little cogroup, e.g., containing a TPP, as illustrated in Fig. 8(a). We refer to the two points where the sphere is intersected by the rotation axis as the south and north pole. Let $N$ and $N_{occ}$ be the total number of bands and the number of occupied bands, respectively. We assume the system to have space-time inversion symmetry $\mathcal{P}\mathcal{T}$ satisfying $(\mathcal{P}\mathcal{T})^2 = +1$, such that there is a basis in which the corepresentation of $\mathcal{P}\mathcal{T}$ is the identity matrix and the Bloch Hamiltonian a real symmetric matrix. Let further $D_0$ and $D_1$ label the symmetry representations of the occupied bands in that basis at the south and north poles of the spherical surface, respectively. In Appendix B1 we show that the Wilson-loop operator $W(\phi)$ computed on the path

$$\Gamma(\phi) = \gamma(\phi)^{-1} \circ \gamma(0)$$

illustrated in green in Fig. 8(a) is constrained by $C_n$ symmetry:

$$W\left(\phi + \frac{2\pi}{n}\right) = D_0(C_n)P(\phi)^1D_1(C_n)^1P(\phi)W(\phi),$$

where $P(\phi) \in \text{SO}(N_{occ})$ is defined by parallel transport [see Eq. (B17) in Appendix B1]. Note that in Eq. (8), one first traverses the path appearing to the right of the composition symbol “$\circ$.”

For arbitrary $N_{occ}$, we consider the implication of Eq. (9) for the Berry phase of the occupied bands on the contours $\Gamma(\phi)$. The Berry phase is given by $\varphi = \arg \det W[79]$, such that

$$\varphi\left(\phi + \frac{2\pi}{n}\right) = \varphi(\phi) + \arg \det[D_0(C_n)D_1(C_n)^1] \mod 2\pi.$$

Due to $\mathcal{P}\mathcal{T}$ symmetry, $\Delta\varphi = \arg \det[D_0(C_n)D_1(C_n)^1]$ is quantized to 0 vs $\pi$. If $\Delta\varphi = \pi$, there are an odd number of NLs in the principal gap crossing the surface in each sector $[\phi, \phi + 2\pi/n]$ [cf. Fig. 8(b)]. This implies that the principal gap is necessarily closed somewhere on the enclosing surface, thus preventing one from assigning a monopole charge to the enclosed TPP. We will see in Sec. IV C that this condition also prevents the corresponding TPP$s$ from exhibiting the higher-order signature at the hinges.

In the remainder of this subsection, we call a TPP admissible when the principal gap on the enclosing sphere can be open. This corresponds to the case with $\Delta\varphi = 0$, which is equivalent to requiring

$$\det[D_0(C_n)D_1(C_n)^1] = 1.$$ 

By our initial assumption, the two occupied bands involved in the TPP are separated from lower-lying occupied bands by an energy gap on the whole surface, such that we can ignore
TABLE II. Bulk-hinge correspondence for triple-point pairs (TPPs) in spinless systems. Triple points (TPs) can arise only in crystals with rotational symmetry $C_n$ (or screw symmetry) of order $n \in \{2, 3, 4, 6\}$; this fixes the nanowire geometry (see table footnote a) in which we study the hinge charges. In particular, the TPs occur along high-symmetry lines (HSLs) with little cogroup (LCG) that has the same rotational symmetry $C_n$ supplemented with space-time inversion ($PT$) symmetry or with mirror ($m$) symmetry with respect to plane that contains the HSL or with both $PT$ and $m$. Note that $C_n$ may be generated by an unantiferro rotational symmetry $C_{n\alpha};PT$ for even $n$, and that the antiferro rotations $C_{n\alpha};PT$ and $C_{n\alpha}PT$ can stabilize TPs even without additional symmetries. (For an easily navigable summary of all admissible symmetry combinations supporting spinless TPs, see Table I.) In the second row we indicate representative HSLs with the required rotational symmetry, which are realized in SGs with a prismatic Brillouin zone (however, the below-listed values of $\Delta Q$, $\chi$, and $w_2$ apply equally to all HSLs with the specified symmetry). In the third row we indicate the generator of the LCG rotational symmetry, i.e., the maximal (unitary or antiunitary) rotational symmetry. The next row lists the possible pairs of TP types along the corresponding HSL which can exhibit a gapped spectrum on the specified symmetry). In the third row we indicate the generator of the LCG rotational symmetry, i.e., the maximal (unitary or antiunitary) rotational symmetry. The next row lists the possible pairs of TP types along the corresponding HSL which can exhibit a gapped spectrum on the specified symmetry. In the third row we indicate the generator of the LCG rotational symmetry, i.e., the maximal (unitary or antiunitary) rotational symmetry. 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with the TP pair are defined as the characteristics of the 2D cut in high-symmetry line, with the 2D irreducible corepresentation (ICR) $\Delta_1$ independent of momentum, and will therefore locally deviate from below $\mu$ two 1D ICRs bulk-boundary correspondence of TPPs, listed in the bottom mulas from Secs. IV A and IV B to derive the higher-order unimportant). Finally, we apply the symmetry-indicator formulas from Secs. IV A and IV B to derive the higher-order bulk-boundary correspondence of TPPs, listed in the bottom of Table II.

Choosing $k_z$ along the HSL and taking 2D cuts of the system at constant $k_z$, we obtain a series of 2D systems with Hamiltonian $\mathcal{H}_k(k_z, k_y)$, which we assume to be at half-filling. This fixes the principal gap to be the second one (such that principal nodes are indicated in red, cf. Fig. 9). Upon increasing $k_z$, the system goes from having $\rho^{2D}$ occupied (to the left of the first TP) to instead having $(\rho_a^{1D}, \rho_b^{1D})$ occupied (to the right of the second TP). Let us refer to the three ranges of $k_z$ separated by the two TPs by the corresponding color of the central NL as orange, red, and blue $k_z$ range. The corresponding band inversions lead to changes in the symmetry indicators $\#\Pi_p^{(n)}$, and thus potentially alter both the corner charge [cf. Eq. (4)] and the 2SW class [cf. Eq. (6)] of the 2D cuts. Let us remark that, in practice, the physical chemical potential has a value independent of momentum, and will therefore locally deviate from the $\mu$ defined above. Nevertheless, generically, the system will still be at half-filling for extended parts of the orange and blue regions which lie far enough from the TP pair. The differences $\Delta Q$, and $\Delta w_2$ are therefore still well defined and unchanged compared to the situation with variable $\mu(k_z)$.

We briefly explain how to apply the 2D symmetry-indicator formulas to 3D systems with $\mathcal{PT}$ and arbitrary $C_n$ symmetry. For concreteness we assume the rotation axis to be along $k_z$. In this case, any 2D cut perpendicular to $k_z$ through the 3D BZ inherits both of these symmetries. In particular, within the 2D plane $\mathcal{PT}$ acts as $(C_2)^{2D}$ with $(C_2)^{2D} = C_2$ being the rotation around the $k_z$ axis, and $T^{2D} = \mathcal{PT} C_2 T = m_z T$ [49] being the composition of the physical time-reversal symmetry with the horizontal mirror symmetry $m_z: z \mapsto -z$. Note that the HSPs entering the symmetry-indicator formulas need to be identified with the intersection of the corresponding HSLs in the 3D BZ with the chosen 2D plane at fixed $k_z$. For $\Gamma^{(n)}$ we thus need to consider the $C_n$-invariant HSLs, while the 2D TRIM correspond to lines invariant under $T^{2D}$. The computed corner charges in the 2D cuts therefore imply the corresponding values of hinge charges in the 1D hinge BZ, while the jump of the 2SW class between two 2D cuts corresponds to the 2SW monopole charge as we explained in Sec. III A and illustrated in Fig. 4.

The hinge charge is only well defined for values of $k_z$, where the bulk of $\mathcal{H}_k$ is gapped and the surface charge vanishes [28]. Similarly, the monopole charges are only well defined as long as there is a surface enclosing the TPP that is not penetrated by NLs in the principal gap (red). While these conditions generally depend on the model parameters, we can formulate the following criteria for a gapped bulk, which conversely implies constraints on the admissible TPP configurations (to be precise, we call a combination of a 2D and two 1D ICRs an admissible TPP configuration if it is not necessarily gapless in the orange or blue $k_z$ range):

(1) In Sec. IV B we have discussed a condition [summarized by Eq. (11) and derived in Appendix B], that the representations of $C_n$ in the orange and blue $k_z$ ranges must necessarily fulfill in order for the TPP to be admissible. According to Fig. 9, we have $D_0(C_n) = \rho^{2D}(C_n)$ and $D_1(C_n) = \rho_a^{1D}(C_n) \oplus \rho_b^{1D}(C_n)$, such that the condition for the TPP configuration to be admissible is

$$\det \rho^{2D}(C_n) = \rho_a^{1D}(C_n) \rho_b^{1D}(C_n).$$

Note that this is fully determined by the rotation eigenvalues since the determinant on the left is just the product of eigenvalues. In Appendix B 4, we show that this excludes exactly the TPPs with two 1D ICRs that have different rotation eigenvalues, i.e., for the little cogroups $C_{6(e)}$ these are the combinations $(E; A, B)$ and for $C_{6(v)}$ the combinations $(E_i; A, B), i = 1, 2$ (we have omitted subscripts of the 1D ICR labels since the argument is insensitive to them). In these cases neither the jump of the hinge charge nor the Euler and 2SW monopole charges are defined.

(2) For the little cogroup $C_{6(e)}$, the gaplessness can be understood from the NL structure implied [60] by the type of TPs involved, as illustrated in Fig. 10. A TPP consisting of one type-A and one type-B TP necessarily has NL arcs in the principal gap that extend beyond the red $k_z$ range. In contrast, if both involved TPs are of the same type, the orange and the blue $k_z$ ranges can generally be gapped. On the one hand, the case of two type-A TPs is very simple since there are no additional NLs and the bulk is gapped in the corresponding regions of $k_z$. On the other hand, for two type-B TPs there must be NL arcs in the principal band gap attached to both TPs. However, the NL arcs can tie the two TPs together in the red $k_z$ range, where the gapless 2D cuts are not considered when analyzing the higher-order topology, thus leaving the orange and the blue $k_z$ range gapped. Note that in the applicable case, i.e., $C_{6(e)}$ which are the only point groups where both types of TPs are possible, this criterion turns out to be equivalent to the first.

(3) While the above two points give necessary criteria for having a gapped bulk, they are not sufficient. Two type-A

FIG. 9. Convention for defining the jump of the fractional hinge charge ($\Delta Q$) and of the second Stiefel-Whitney monopole ($\Delta w_2$) associated with a pair of triple points (TP, yellow dots) in a four-band configuration. The black lines indicate the band structure along a high-symmetry line, with the 2D irreducible corepresentation (ICR) $\rho^{2D}$ passing from the bottom (orange) to the central (red) to the upper (blue) energy gap with increasing momentum $k_z$ due to crossing two 1D ICRs $\rho_a^{1D}$ and $\rho_b^{1D}$. The green dashed line ($\mu$) indicates half-filling at various $k_z$. The quantities $\Delta Q$ and $\Delta w_2$ associated with the TP pair are defined as the characteristics of the 2D cut in the region where $\rho^{2D}$ is unoccupied (i.e., above $\mu$) from which we subtract the characteristics of the 2D cut in which $\rho^{2D}$ is filled (i.e., below $\mu$). In practice, the physical chemical potential has a value independent of momentum, and will therefore locally deviate from the $\mu$ defined above. Nevertheless, generically, the system will still be at half-filling for extended parts of the orange and blue regions which lie far enough from the TP pair. The differences $\Delta Q$, and $\Delta w_2$ are therefore still well defined and unchanged compared to the situation with variable $\mu(k_z)$.
TPs do not have any NL arcs attached, but they are often accompanied by nexus points, i.e., points on the HSL away from the TPs where NL arcs coalesce [59] [see Figs. 11(a) and 11(b)]. If there are an even number of nexus points in the principal gap, then there are two options: (a) the NL arcs connect together through the red \( k_z \) range or (b) the NL arcs extend outside the red \( k_z \) range, making the orange and blue \( k_z \) ranges gapless. These two cases are illustrated in Figs. 11(a) and 11(b), respectively, for a \( C_n \)-symmetric example. Similarly, the NL arcs of two type-B TPs might not connect through the red \( k_z \) range as indicated in Fig. 10(b) but rather extend outside of it as shown in Fig. 11(c). These cases are not distinguished by symmetry properties but by the model parameters. The results of our analysis, e.g., Table II, apply to the cases that do have a gapped bulk in some part of both the orange and the blue \( k_z \) ranges.

Let us remark that the cases disallowed by the first criterion for point group \( C_{6v} \) (which according to Table I involve a pair of type-A TPs) correspond to situations where there is one (or a larger odd number of) symmetry-imposed nexus points of NLs in the principal gap, i.e., with the NLs attaching to the red region demarcated by the two TPs. An example of such a TPP configuration is illustrated in Fig. 8(b). Since an odd number of nexus points cannot be paired as in Fig. 11(a), there necessarily exist extended NLs which render either the orange or the blue \( k_z \) region gapless. Therefore, the corresponding TPP is not admissible for the same reason as is visualized for the mixed-type TPP in Fig. 10(c).

Having clarified the necessary conditions to realize an admissible TPP, let us tackle their associated hinge-charge jump. To observe the hinge charge, the system needs to be extended in the \( z \) direction and finite in the \( x \) and \( y \) directions, with a geometry possessing the same \( C_n \) symmetry as the SG [see Fig. 7(a)]. We need to distinguish geometries with the center of the rotational symmetry being placed at different WPs in the unit cell. In Appendix A 3 we consider all possible cases for each combination of ICRs listed in Table II and compute the hinge-charge jump using the appropriate symmetry-indicator formulas [30] [in particular, aside from Eqs. (4a) and (4b), we also need the analogous expression for \( Q^{(3)} \); see Eq. (A1)]. Note that for this analysis the ionic charge distribution is irrelevant because it does not depend on \( k_z \) and therefore it does not contribute to the jump of the hinge charge. Table II summarizes the results of this analysis. We observe that the combination of ICRs uniquely determines the jump of the hinge charge. In particular, there is a nonvanishing jump \( \Delta Q \neq 0 \mod e \) quantized into multiples of \( \frac{\xi}{n} \) for \( C_n \) symmetry for any TPP.

Let us briefly comment on the jump of the surface charge. As already stated, the vanishing of the fractional part of the surface charge (which is related to bulk polarization [80]) is a necessary condition for the hinge charge to be observable [28]. Therefore, to observe the hinge-charge jump, the surface charge must vanish for the \( k_z \) ranges on both sides of the TPP, which can only happen if the TPP is not associated with a fractional jump \( \Delta P \), \( \Delta P \mod eR \) (where the Bravais vectors \( R \) constitute the usual ambiguity of bulk polarization [81]) for all tabulated TPs. Therefore, the surface charge does not present an obstacle for the definition of the hinge charges, and we expect the hinge-charge jump to be observable for an appropriate choice of the boundary termination.

To compute the jump of the 2SW class, or equivalently the 2SW monopole charge \( w_2 = \Delta w_2 \) carried by the red NL segment, we proceed as follows. For systems with \( C_4 \) or \( C_6 \) symmetry the 2SW class of the 2D cuts can be computed readily by applying Eq. (6) with the appropriate interpretation of the HSPs, as described above. The full derivation can be
found in Appendix A3 and the results are displayed in the bottom-most row of Table II. Consistent with the results of Sec. III A, we find that type-(A, A) TPPs in \(PT\)-symmetric systems universally carry \(w_2 = 1\). Furthermore, we recognize the following correspondence principle between the bulk invariant \(w_2\) and the hinge signature \(\Delta \bar{Q}_\ell\) (which is only defined modulo \(e\)): a nontrivial 2SW monopole charge \(w_2 = 1\) implies a fractional hinge-charge jump of the minimal nonvanishing magnitude \(\Delta \bar{Q}_\ell = \pm \frac{\pi}{e}\), while \(w_2 = 0\) results in a twice as large a jump \(\Delta \bar{Q}_\ell = \pm \frac{2\pi}{e}\).

Determining the 2SW monopole charge in the case of \(C_3\) symmetry is not as straightforward. However, we note that the 2SW monopole charge is attributed to the red NL segment along the HSL as illustrated in Fig. 3(b) and is therefore a feature local in \(k_x, k_y\). Thus, it cannot depend on the specific choice of HSL in the BZ, but only on the Hamiltonian near the HSL. Noting that the little cogroup of all three HSLs has the same rotational symmetry and there is only one class of combinations of ICRs, the admissible values of the 2SW monopole charge \(w_2\) are the same for all three HSLs \(\Gamma A, KH, K' H'\). In the next paragraph we argue that, in fact, the 2SW class is not symmetry indicated in the \(C_3\)-symmetric case, meaning that both \(w_2 = 0\) or 1 are possible. We emphasize that this is not in contradiction to the bulk-hinge correspondence principle described above because the fractional part of the hinge-charge jump satisfies \(\pm \frac{\pi}{2e} = \mp \frac{2\pi}{e}\) mod \(e\). Thus, the hinge signatures of nontrivial and trivial 2SW monopole charge become indistinguishable.

The fact that the 2SW class is not symmetry indicated in a SG with \(C_3\) symmetry can be easily deduced from the other results in Table II. In particular, note that a SG with \(C_6\) symmetry also has \(C_3\) symmetry. Thus, we can deform any of the possible TPP configurations on the \(\Gamma A\) line of a sixfold-symmetric system (cf. last two columns of Table II), having either \(w_2 = 0\) or 1, into a TPP configuration of a \(C_3\)-symmetric system by introducing a small \(C_2\)-breaking perturbation. However, Table II shows that in the in threefold-symmetric little cogroups, only a single combination of ICRs is possible, such that any initial choice of the TPP in the \(C_6\)-symmetric case results in that unique TPP type of the \(C_3\)-symmetric system (in particular, type-A TPPs generically transform into type-B TPPs). Since the 2SW class requires only \(PT\) symmetry (which is preserved when breaking \(C_2\)) and the 2D cuts outside the red \(k_x\) range remain gapped under the addition of a small perturbation, the 2SW class is unaffected by the perturbation. This implies that both \(w_2 = 0\) or 1 are possible for TPPs in \(C_3\)-symmetric SGs, and that the 2SW class is not symmetry indicated. We demonstrate this feature for two explicit models in Sec. V D.

The symmetry-indicator formula for the Euler class, Eq. (13), is, in contrast to the other formulas, already formulated in 3D. It involves the corepresentations of \(C_n\) in the orange and blue \(k_z\) ranges. By going through all allowed combinations of ICRs (cf. Appendix B4), we verify that indeed \(\rho^{3D}(C_n)\) and \(\rho^{1D}(C_n) \oplus \rho^{1D}(C_n)\) are \(SO(2)\) matrices; then we extract \(r_0 = r_{2D}, r_1 = r_{1D+1D}\) and compute \(\chi\). The results are shown in the second to last row of Table II for the cases with \(PT\) symmetry. We observe that in all cases where it is defined, the Euler monopole charge is nontrivial and consistent with the independently calculated \(w_2\), via the relation \(w_2 = \chi\) mod 2. Note that for \(n = 3\), \(\chi\) is determined only modulo 3 and thus has undetermined parity, which is consistent with the 2SW not being symmetry indicated in that case (cf. Sec. V D).

Finally, we remark on the consistency of the results in Table II for a TPP on the \(KH\) line of a \(C_6\)-symmetric compared to a \(C_3\)-symmetric system. Naturally, a system with sixfold rotational symmetry is also threefold rotation symmetric, such that one expects compatibility of the results for the two cases. However, there are two caveats: (1) in a \(C_6\)-symmetric system the \(KH\) and \(K'H'\) HSLs are equivalent such that there are in fact two symmetry-related TPPs per BZ at the same value of \(k_x\), and (2) the hinge-charge jumps in the two cases are computed for a different geometry of the sample [cf. Fig. 7(a)]. Therefore, if we only consider the \(C_3\) symmetry of a \(C_6\)-symmetric system, we have to (1) count contributions of identical TPPs on the two HSLs \(KH\) and \(K'H'\), and (2) deform the sample with hexagonal cross section into one with a triangular cross section by combining two corners into a single new corner as depicted in Fig. 7(b).

With this insight, it is easily checked that the corresponding entries in Table II are fully consistent. First, for the 2SW class the two monopole charge contributions are additive, \(w_2^{(3)} = 2w_2^{(1)}\), which results in \(w_2^{(6)} = 0\ mod 2\) for both \(w_2^{(3)} = 0\ or 1\). Furthermore, the corner charge of the triangular cross section \(Q_{\ell h}^{ab}\) is given by the sum of two of the corner charges of the hexagonal cross section \(Q_{\ell h}^{ab} = Q_{e}^{a} + Q_{a}^{b}\) [cf. Fig. 7(b)]. Note that due to the sixfold rotational symmetry \(Q_{e}^{a} = Q_{a}^{b} = \frac{\chi}{e}\ mod e\), such that for the \(C_6\)-symmetric model with a TPP on \(KH\) in the triangular geometry we find \(Q_{\ell h}^{ab} = 2\frac{\chi}{e}\). On the other hand, when interpreting the same model as being \(C_3\) symmetric, we simply add the corner charges for a TPP on \(KH\) and \(K'H'\), giving \(Q_{\ell h}^{ab} = 2\frac{\chi}{e}\) as well.

D. Effect of symmetry breaking

The discussion in Sec. IV C has focused on spinless systems with \(PT\) symmetry (corresponding to the MPGs in rows two and four of Table I), which has allowed us to characterize the TPPs with the Stiefel-Whitney monopole charge. However, stable TPPs can exist even when the \(PT\) symmetry is removed [59] (cf. Table I); in this case, the monopole charges cease to exist, but the bulk-hinge correspondence of the TPPs persists. In this section we discuss the effect of symmetry breaking on the derived bulk-hinge correspondence of TPPs. First, in Sec. IV D 1 we argue that the hinge-charge jumps derived for the cases with \(m_\ell\) and \(PT\) symmetry still apply when the \(PT\) symmetry is broken while \(m_\ell\) remains present. We continue in Sec. IV D 2 with a discussion how the derived results generalize to the cases where the TPPs are protected by the antiunitary \(C_6 PT\) rotational symmetry. Finally, in Sec. IV D 2 we briefly analyze the effect of breaking other combinations of symmetries, which generally leads to the loss of TPPs and to the formation of other species of band nodes. Our results are summarized in Table III.

1. Triple points protected by \(C_n\) and mirror symmetry

We first discuss the effect of breaking \(PT\) symmetry while keeping the rotational symmetry \(C_n\). According to Table I, mirror symmetry \(m_e\) is then required to protect TPPs. The crucial observation is that if both \(PT\) and mirror \(m_e\) sym-
TABLE III. Effect of symmetry breaking on triple-point pairs (TPPs). We initially consider TPPs in the combined presence of PT (space-time inversion), Cn (rotation of order n ∈ {3, 4, 6}), and mv (vertical mirror) symmetries, corresponding to the first row of the table. Such TPPs are characterized by the second Stiefel-Whitney (2SW) monopole, by symmetry indicators (#,/), and by the fractional hinge-charge jump (integer multiples of e/n). We then consider the breaking of the various symmetries, as analyzed in Sec. IV D. We find that TPPs can evolve into higher-order Weyl points (HO-Weyl), into nodal lines (NLs) with the 2SW monopole, or into Weyl points or nodal lines without higher-order topology (indicated as “various”).

| PT | Cn | CnPT | mv | Nodes | Bulk invariant | Hinge charge |
|----|----|------|----|-------|--------------|-------------|
| √  | √  | √    | (√) | TPPs  | 2SW, #(m)     | e/n Z        |
| ×  | √  | ×    | (√) | TPPs  | #(m)         | e/n Z        |
| ×  | Cn/2 | ×  | (√) | TPPs  | #(m)         | 2e/n Z       |
| √  | ×  | ×    | (√) | NLs   | 2SW          | Not quantized|
| ×  | ×  | ×    | (√) | HO-Weyl| #(m)        | e/n Z        |
| ×  | ×  | ×    | (√) | (Various) | —            | Not quantized|

The requirement of the presence of Cn/2 restricts n to 4,6.

symmetries are present in the little cogroup, then the ICRs are not modified by the removal of PT [82,83], i.e., the ICRs of the unitary symmetries of the full group are exactly given by the ICRs of the unitary subgroup. As a consequence, the classification of TPPs in systems with mv symmetry based on ICRs is identical both with and without PT symmetry; in fact, detailed analysis [59] reveals that the type (A vs B) produced by the crossing of specified ICRs is also unaffected by the removal of PT. An analogous statement also applies to the result that the ICR combination (C,PT) is necessarily gapless (see Appendix B5).

To derive the hinge-charge jumps ΔQ associated with TPPs protected by mv symmetry without PT, we should, in principle, repeat the above-described analysis (detailed in Appendix A5) with the symmetry-indicator formulas that do not assume time-reversal symmetry, i.e., (A1)–(A3), and the ICRs of the point groups without PT symmetry. However, as described in the previous paragraph, the ICRs (and therefore the rotation eigenvalues) are identical to the ICRs of the corresponding point groups with PT symmetry, such that Eqs. (A2) and (A3) still simplify to Eqs. (A4) and (A5). This implies that the jumps in the symmetry indicators are not changed when breaking PT symmetry while keeping the rotational symmetry Cn, and the hinge-charge jumps ΔQ remain unaltered as well. On the other hand, the monopole charges are not defined in the absence of PT symmetry. Therefore, all results in Table I except for the last two rows apply to systems with mirror mv symmetry but no PT symmetry.

2. Triple points protected by the antiunitary CnPT symmetry

Since TPPs can also be protected by the antiunitary rotational symmetry CnPT (cf. Table I), PT symmetry can alternatively be broken while keeping CnPT. In such a case, the Cn rotational symmetry is broken, while Cn/2 = (CnPT)2 is a symmetry of the system. We have to distinguish two scenarios: the TPPs are either protected by CnPT or by CnPT. Note that, as we discuss in Appendix B5, Eq. (14) still applies in these MPG, yet a careful analysis reveals that this constraint does not imply the inadmissibility of any TPP configurations.

We begin with analyzing the case of CnPT, where the largest remaining rotational symmetry is C3; therefore, a triangular geometry needs to be considered and the relevant rotational symmetry quantizing the hinge charges is C3. Furthermore, we find [82,83] that the corresponding MPGs with and without mv symmetry (6, 2m′2 and 6′, respectively) have the same unitary subgroup as the PT-symmetric MPGs 3m and 3′, respectively, with matching ICRs. As a consequence, the hinge-charge jump is the same as for the other little corgroups with C3 rotational symmetry, i.e., no change in the bulk-boundary correspondence. This has motivated us to group C3 and CnPT within a single column of Table II. We remark, however, that although the ICRs of the subgroup and the higher-order bulk-boundary correspondence are equivalent to the C3 case, this is not true for the corresponding TP types, which depend on the ICRs of the full point group. Irrespective of the presence (MPG 6, 2m′2) vs absence (MPG 6′) of mv symmetry, the TPPs protected by CnPT are always type A [59] In the latter case, this simply follows from the absence of symmetries (no mv and no PT) that can protect NLs lying off the rotation axis, while in the former this requires a more in-depth analysis [59].

Similarly, C4 and PT can be broken while keeping CnPT. However, in that case the largest remaining rotational symmetry is C2, such that in a square geometry only the sum over two adjacent hinges gives a quantized charge [28]. The resulting little corgroups are the MPGs 4 2m (with mv mirrors) and 4 (without mv mirrors), which are subgroups of the PT-symmetric MPGs 4/m, 4/m′ and 4/m′′, respectively. It is easily verified [82,83] that all four listed MPGs have equivalent C2-return eigenvalues for the 1D and 2D ICRs: all 1D ICRs are even while all 2D ICRs are odd under C2. Since in the presence of CnPT the hinge-charge jump is completely determined by C2-return eigenvalues, the hinge-charge jump of TPPs protected by CnPT is, in principle, the same as in the C4 case. However, since only the sum of charges on two adjacent hinges is quantized, the resulting jump is doubled to ΔQ = 2 × mod e = mod e. The TPPs protected by CnPT are always type A [59], i.e., of the same type as before the PT breaking. With this analysis, we explained the “C2” column in Table II, and established the higher-order bulk-boundary correspondence for all TPPs listed in Table I.

3. Breaking the symmetry protection of triple points

Aside from breaking the symmetry in ways that keep the TPPs robust, here we briefly discuss the effect of breaking symmetries that protect the TPPs. We find that this generically results in the conversion of the TPPs to other species of band nodes [84]. The case of broken Cn symmetry (with or without mv) in the presence of PT symmetry has already been discussed implicitly in Sec. III A for type-(A, A) TPPs, where we revealed their conversion [60] into multiband nodal links carrying a nontrivial 2SW monopole. Using the results in Table II, we can now extend this discussion to generic TPPs. If the TPP carries w2 = 1, then the 2SW monopole implies stable multiband nodal links upon breaking the rota-
tional symmetry. On the other hand, note that \( w_2 = 0 \) only arises for type-(B, B) TPPs. Since these are characterized by the attached NL arcs carrying a \( \pi \) flux of Berry phase [85], and this quantization is unaffected by the broken rotational symmetry, a small \( C_n \)-breaking perturbation leaves behind a NL composition with a trivial 2SW monopole. In both cases, \( w_2 \in \{0, 1\} \), the absence of rotational symmetry implies the absence of the hinge-charge quantization for all geometries depicted in Fig. 7.

We next analyze the situation where \( C_n \) is kept but both \( m_v \) and \( PT' \) are broken. In such cases, the rotational symmetry ensures that the quantized hinge-charge jump associated with the TPP is maintained. At the same time, it is impossible to protect NLs (including the 2D ICR along the HSL) without \( PT' \) and \( m_v \) [86] using \( C_n \) alone, and instead Weyl points [87] become the generic band degeneracy. Therefore, the breaking of both \( m_v \) and \( PT' \) symmetry results in a higher-order Weyl semimetal with Weyl points along the rotation axis [40–42], characterized by quantized hinge-charge jumps.

We remark that in spinless systems higher-order Dirac points [9,45–47] cannot be obtained by perturbing a TPP; and vice versa, a TPP cannot be created by perturbing a higher-order Dirac point. Nonetheless, the results in Table II readily characterize the quantized hinge-charge jumps.

In the previous section we have shown that TPP configurations demarcate a NL segment that can be characterized by an Euler and 2SW monopole charge (if \( PT' \) is present) and by a fractional hinge-charge jump (for all cases). Here we verify these theoretical predictions by analyzing several concrete tight-binding models: First, in Sec. VA we revisit the \( C_4 \)-symmetric model introduced in Sec. II, and we relate the phenomenology described there to the theoretical results presented in Sec. IV. Subsequently, in Secs. VB and VC we present two \( C_6 \)-symmetric models, one involving type-A and the other involving type-B TPPs, and confirm that the jumps in the 2SW class and in the hinge charge as well as the Euler monopole charge follow the predictions of Table II.

For simplicity, all the discussed models retain both the (spinless) \( PT' \) symmetry and the mirror \( m_v \) symmetry. It follows from Table I and from the subgroup relations discussed therein that models for all other species of TPPs can in principle be obtained by applying an appropriate perturbation to one of the \( C_4 \) or \( C_6 \) models discussed in the following subsections. We utilize this feature in Sec. VD, where we break the \( C_2 \) symmetry in each of the two \( C_n \)-symmetric models. This construction allows us to explicitly show that the 2SW class is not symmetry indicated in \( C_3 \)-symmetric systems, as previously stated (but not proved) in Sec. IV C.

A. \( C_4 \)-symmetric model

In Sec. II we introduced a tight-binding model with hinge charges induced by a NL configuration with two pairs of TPs in adjacent band gaps [see Eq. (1) and Figs. 1 and 2]. We observed that the red NL segments divide the BZ into two parts: one with nontrivial 2SW class on 2D cuts through the BZ and hinge charge \( \frac{\pi}{2} \), and another with trivial 2SW class and a vanishing hinge charge. We now recast the phenomenology observed for that model in light of the bulk-hinge correspondence derived in Secs. III and IV and summarized in Table II. In particular, we recognize that the 2SW class and hinge charge are consequences of the nodal configuration of the model with the robust signatures being their jumps as a function of \( k_z \). In addition, we also clarify how the hinge charge \( Q(k_z) \) plotted in Fig. 2(b) has been extracted.

As we argued in Sec. III A and proved using symmetry indicators in Sec. IV C, each four-band TPP along a \( C_4 \)-rotation axis (which are automatically type A) demarcates a NL segment in the principal gap [red in Fig. 12(a)] which carries 2SW monopole charge \( w_2 = 1 \). This can be diagnosed by computing the Wilson-loop spectrum of the lower two bands on an ellipsoid [purple in Fig. 12(a)] containing one such NL segment. Figure 12(b) shows that there is a single winding, confirming that indeed \( |\chi| = 1 \) and \( w_2 = 1 \).
than a unit cell, we observe strong oscillations, which make it impossible to directly integrate the charge on a corner or even detect any possible localization. This is a typical problem for the case of ionic crystals and is usually tackled by coarse graining the charge distribution \[29,30,89\]. We perform a discrete version of such a coarse graining by following a scheme explained in Appendix D1. Considering each orbital position (i.e., the two per unit cell) as a separate site of a square lattice, we compute the charge on the dual square lattice [cf. Fig. 23(b)] by distributing charge on each site of the original lattice with equal weights to the nearest sites of the dual lattice. Effectively, this coarse grains the charge distribution to the length scale of one unit cell and significantly reduces the oscillations, as shown in Figs. 13(c) and 13(d).

After coarse graining, we can integrate over various regions to find the bulk, edge, and corner charges. First, we observe that the bulk and edge charges vanish for both \(k_z = 0, \pi\) as can be seen in Figs. 13(c) and 13(d). Due to the double-band inversion at \(\Gamma\), the model has vanishing Berry phases along the path \(M\Gamma M\) (perpendicular to the edge), which implies \[80\] that the bulk polarization \[81\] and therefore the edge charge vanish. On the other hand, the corner charge only vanishes for \(k_z = \pi\). The nonvanishing corner charge at \(k_z = 0\) is a consequence of the corner-induced filling anomaly \[28\]. This excess charge is strongly localized near the four corners. Integrating over the gray area indicated in the figure, and taking care that the integration region forms 90° angles with the edges \[29\], we find \(Q_c = 0.2498e\) for \(k_z = 0\) and \(Q_c = 8 \times 10^{-9}e\) for \(k_z = \pi\). The deviations from the expected values \(\frac{\pi}{2}\) and 0 are due to finite-size effects, and can be further reduced by increasing the total system size and the coarse-graining scale while keeping the relative size of the integration region fixed.

We numerically compute the 2SW class and the (coarse-grained) corner charge of the \(C_4\)-symmetric model defined in Eq. (1) using the described methods for planes at multiple values of fixed \(k_z\). Our results are summarized in Fig. 2(b) in Sec. II. We find that the model exhibits a jump of the 2SW class by +1 and of the hinge charge by +\(\frac{\pi}{2}\) as the 2D ICR moves from the occupied to the unoccupied band subspace. This agrees with the prediction of Table II since the ICRs of the bands involved in the two TPs on the HSL \(\Gamma Z\) are \((E; B_1, B_2)\). While far away from the TPs the hinge charge is very close to the quantized value, there are finite-size effects. This is especially observed in the small deviations from the quantized values for \(k_z\) near to the closing of the principal gap (i.e., in the vicinity of each TP), where the localization length of the corner charge is expected to grow.

### B. \(C_4\)-symmetric model with type-A triple points

To realize a type-(A, A) TPP along a \(C_4\) rotational symmetry, we consider the \(\Gamma A\) line of the hexagonal SG \(P 6/mmm\) (No. 191). More specifically, we consider a model [detailed in Eq. (C3) of Appendix C2a] with \((d_{x^2}, d_{y^2}-z^2})\) orbitals transforming in the 2D ICR \(E_2g\) and orbitals transforming in 1D ICRs \(B_{1u}\) and \(B_{2u}\), respectively, all placed at the Wyckoff position 1a with site-symmetry group \(D_{4h}\). We tune the parameters such that the \(d\) orbitals have lower energy than the \(f\) orbitals at all HSPs with the
exception of a double-band inversion at $\Gamma$. Consequently, on $\Gamma A$ two 1D ICRs ($B_1$, $B_2$) consecutively cross the 2D ICR ($E_2$) resulting [60] in two type-$A$ TPs. The band structure and the NL configuration of the model are displayed in Figs. 14(a) and 14(b), respectively. We remark that apart from the twofold degeneracies along the $H\Gamma$ lines; however, these lie within the occupied band subspace and therefore have no effect on the discussed topological features. The model exhibits no additional NLs beyond these degeneracies along the HSLs. We remark that for the computation of the hinge charges we set the compensating ionic charge to also reside at site 1.

According to Table II, we expect a jump of $+\frac{e}{6}$ in the hinge charge and $+1$ in both the Euler and 2SW class when going from the orange $k_z$ range to the blue $k_z$ range. More precisely, based on a symmetry eigenvalue analysis and Eqs. (4) and (5), we expect that the 2SW class is 1 in the blue $k_z$ range and 0 in the orange $k_z$ range, while the hinge charge should be $\frac{e}{6}$ and 0, respectively. The results for the 2SW class are verified by computing the Wilson-loop spectra of the lower two bands on horizontal cuts through the Brillouin zone parametrized by the projection $k_z$ of the momentum onto the first reciprocal lattice vector. Blue/orange lines show the spectrum for $k_z = 0$ (single winding) and green/red lines for $k_z = \pi$ (no winding).

To verify the results for the hinge charge, we construct a system finite in $x$ and $y$ directions with 16 hexagonal shells in the cross section [the cross section illustrated in Fig. 14(d) has three shells]. Using exact diagonalization we find the charge distribution at half-filling for 2D cuts of the BZ that lie outside the 2D cross section while it vanishes both in the bulk as well as along the edges. Note that while the charge vanishes on the edges which visually obscure the localization of the corner charge. To reduce these oscillations, we perform coarse graining similar to the one described in the previous subsection. The major technical difference is that here we coarse grain over a hexagonal supercell with two shells, i.e., seven unit cells, in one iteration (cf. Fig. 23). After two iterations we end...
up with a coarse-grained lattice that is smaller by two shells. Integrating over the gray corner area in Fig. 14(e) we obtain a quantized value of the corner charge in (f).

The localization length is larger than for the model shown in Fig. 14, such that finite-size effects produce a visible deviation from the ideal analysis and Eqs. (4) and (5), we anticipate that the 2SW class vanishes in both regions, while the hinge charge is expected to be 0 and \(-\xi\) in the orange and blue \(k_z\) range, respectively, assuming that the compensating ionic charge is placed at position 1a.

We verify these predictions numerically. First, in Fig. 15(c) we plot the Wilson-loop spectra of the lower two bands on horizontal cuts at both \(k_z = 0\) and \(\pi\). Since they both exhibit even winding number, we confirm that \(w_2 = 0\) on both sides of the TPPs. We observe that the Wilson-loop spectrum for the 2D cut at \(k_z = 0\) has winding number \(\pm 2\), meaning that the corresponding 2D model is an Euler insulator [74]. The double winding also implies that each TPP with its attached (red) NL arcs (the nodal-line nexus) carries a Euler class \(|\chi| = 2\) on both the occupied and the unoccupied band subspaces, as predicted. Therefore, as long as \(\mathcal{PT}\) symmetry is present, the only way to gap out the red NL nexus is to annihilate it with the other NL nexus [68]. We remark that this topological obstruction is trivialized in the presence of additional occupied and unoccupied bands [71].

To calculate the hinge charge, we construct a system finite in \(x\) and \(y\) directions with 20 hexagonal shells in the cross section [in Fig. 15(d) we illustrate a system with three hexagonal shells]. By exact diagonalization we find the charge distribution at half-filling for values of \(k_z\) where the spectrum is gapped. In Fig. 15(e) the charge distribution for \(k_z = 0\) is shown. The charge is still localized at the corners of the 2D cross section and vanishes both in the bulk as well as along the edges. However, due to trivial in-gap states and therefore a reduced energy gap, we observe an oscillation of
the charge distribution in the direction perpendicular to the edge, as well as a significantly larger localization length for the corner charge than found in the previous hexagonal model. In fact, the chosen system is too small to achieve convergence, but it is sufficient to support the theoretical predictions in Table II. Integrating the coarse-grained charge distribution over the gray edge area in Fig. 15(e) we obtain $4 \times 10^{-2} |e|$; while over the gray corner area we find $-0.2983e$, which is close to the ideal result $-e$ in the absence of finite-size effects.

We repeat the same analysis for 2D cuts for multiple values of $k_z$, and plot the dependence of the 2SW class and of the hinge charge as a function $k_z$ (where the gap is open) in Fig. 14(f).

D. $C_3$-symmetric models

In this section, we explicitly show that in the presence of $PT$ symmetry there exist $C_3$-symmetric models where the TPPs carry either $w_2 = 0$ or 1. We therefore confirm that the 2SW monopole charge in $C_3$-symmetric SGs is not symmetry indicated, thus justifying the ambiguous entry in Table II. This freedom is present despite the fact that (cf. Table I), $C_3$-symmetric HSLs only support a single species of TPs, namely, type B with three attached NLs arcs and with the central NL carrying Berry phase $\pi$.

We can obtain such $C_3$-symmetric models by reducing the $C_6$ symmetry of the models discussed in Secs. VB and VC down to $C_3$ (while keeping $PT$). A possible perturbation that achieves that is given by Eq. (C6) in Appendix C2c. The resulting NL structure for each parent model is shown in Figs. 16(a) and 16(b) and 16(d) and 16(e), respectively. Note that the 2SW monopole charges of the TPPs in the parent hexagonal models are not changed by the trigonal perturbation: as long as the enclosing ellipsoid [purple in Figs. 16(b) and 16(e)] is chosen to be sufficiently large to contain the lobes of red NLs, the principal gap does not close on that ellipsoid, keeping the Wilson-loop winding invariant. We confirm this by explicitly computing the Wilson-loop spectra on the enclosing ellipsoids of the perturbed models, plotted in Figs. 16(c) and 16(f).

We briefly comment on the change of the NL configurations from Figs. 14(b) and 15(b) to Figs. 16(b) and 16(e), respectively. In both cases, the central NL stretched along $\Gamma A$ initially carries quaternion charge $-1$ (corresponding to Berry phase $2\pi$ [66], i.e., it is a quadratic NL) before switching on the trigonal perturbation. Let us first consider the case of type-A TPs [$w_2 = 1$, Figs. 16(a)–16(c)]. Here, as soon as the perturbation is switched on, all three segments of the central quadratic NL, i.e., in the orange, red, as well as blue $k_z$ ranges, split into four linear NLs with Berry phase $\pi$ each. One NL of the quadruplet is still pinned to the $\Gamma A$ line, while the other three NLs are related by the $C_3$ symmetry and remain attached to the TPs. As a result, the heagonal type-A TPs with no attached NL arcs have transformed into trigonal type-B TPs with three attached NL arcs in each gap, as detailed in Fig. 16(b).

For the hexagonal model with type-B TPs [$w_2 = 0$, Figs. 16(d)–16(f)], the process is similar; in particular, one observes the same splitting of the central quadratic NL into four linear NLs around the HSL. However, in this case the
FIG. 17. Bulk properties of the compound Sc$_3$AlC. The band structure (a) without any strain and (b) with 6.6% uniaxial compressive strain in $z$ direction, which generates a triple-point pair on the $\Gamma Z$ line. Triple points are indicated by yellow arrows. (c) Closeup of the band structure near the triple-point pair with the relevant bands labeled by their irreducible corepresentations. (d) The Brillouin zone of the tetragonal lattice of strained Sc$_3$AlC. The high-symmetry points and mirror planes are indicated. (e) Nodal lines in the relevant three gaps (orange, blue, red according to increasing energy) determined from the Wannier tight-binding model for the mirror planes shown in (d). The triple point is clearly type $A$. The cross sections of the ellipsoid on which we compute the second Stiefel-Whitney monopole charge with the mirror planes are indicated by black ellipses. (f) Wilson-loop spectrum of the relevant bands computed on the ellipsoid indicated in (e); the single winding implies $w_2 = 1$.

hexagonal NL configuration starts out with six attached NLs per gap because the hexagonal TPs have been type $B$. Here the three new NL arcs either annihilate with three of the original NL arcs (in the principal gap, red) or combine with the original NL arcs to form intersecting nodal chains (other two gaps, orange and blue) [90]. As a result, we find that the hexagonal type-B TPs have been transformed into trigonal type-B TPs with three attached NLs per gap, as predicted in Ref. [60]. The intersection of the orange and of the blue NLs visible in Fig. 16(e) is stabilized by the non-Abelian band topology in the presence of $m_v$ and $\mathcal{P}\mathcal{T}$ symmetries, as discussed in Ref. [66].

VI. MATERIAL EXAMPLES

In this section we discuss two concrete material examples that illustrate the introduced phenomenology. While these examples demonstrate that the higher-order topology of TPs can arise in crystalline solids, the large values of strain required to realize the presented band structures imply that our particular materials predictions are not amenable to experimental studies, and that further research is needed to find realistic material candidates. Note that in Sec. VIII we briefly discuss the higher-order bulk-boundary correspondence for TPPs in spinful systems.

Our discussion is structured as follows. In Sec. VI A we show that the compound Sc$_3$AlC subjected to large uniaxial strain exhibits a TPP with type-$A$ TPs on the $Z\Gamma Z$ line and no interfering NLs. Based on first-principles calculations and an ab initio tight-binding model, we compute the 2SW monopole charge and the hinge-charge jump. We find that the 2SW monopole charge takes value $w_2 = 1$ and that a fractional hinge-charge jump $\Delta\chi = \frac{1}{4}$ is present, in agreement with the values predicted by Table II. This demonstrates the higher-order bulk-boundary correspondence introduced in Sec. IV.

In Sec. VI B we study a material example with a NL segment carrying nontrivial Euler monopole charge. The TP material Li$_2$NaN [60,91] has a single pair of inversion-related type-$A$ TPs along the $A\Gamma A$ line. Based on an effective tight-binding model [60], we show that one of the NL segments carries Euler monopole charge $|\chi| = 2$. Furthermore, we demonstrate that this leads to a topological obstruction preventing the removal of that NL segment when colliding the two TPs at the $A$ point, instead leading to a conversion into a nodal ring.

A. Nontrivial Stiefel-Whitney class in strained Sc$_3$AlC

We first consider Sc$_3$AlC [92], which, on the level of a Wannier tight-binding model, manifests the bulk-hinge correspondence for TPPs derived in Sec. IV C. The compound has a cubic crystal structure with SG $Pm\bar{3}m$ (No. 221) and exhibits a threefold-degenerate touching point at $\Gamma$ and TPs on the $\Gamma X$, $\Gamma Y$, and $\Gamma Z$ lines (which are all equivalent) [see Fig. 17(a)]. Furthermore, the spin-orbit coupling is expected to be small due to the elements involved being light, therefore, we can neglect it and treat the electrons as spinless. Then, the system
possesses $PT$ symmetry squaring to $+\mathbb{I}$. Applying uniaxial compressive strain along one of the equivalent crystal axes (which we choose to be the $z$ direction) removes the TPs on the $\Gamma X$ and $\Gamma Y$ lines leaving only those on the $\Gamma Z$ line, and splits the touching point at $\Gamma$ into two additional TPs on the $\Gamma Z$ line [cf. Fig. 17(b) for approximately 6.6% strain]. The result is a configuration of two inversion-symmetry-related TPs on the $\Gamma Z$ line with one TPP shown in Fig. 17(c). The strained material has a simple tetragonal crystal structure with SG $P4/mmm$ (No. 123).

We study the material by first obtaining the band structure and wave functions from density functional theory (DFT) calculations with the projected augmented wave (PAW) method implemented in the Vienna $ab initio$ simulation package (VASP) [93,94] with generalized gradient approximation (GGA) and Perdew-Burke-Ernzerhof (PBE) approximation [95]. We use a $\Gamma$-centered $8 \times 8 \times 8$ $k$ mesh. Uniaxial compressive strain in $z$ direction is modeled by reducing the lattice constant in that direction by the appropriate amount. The lattice structure of Sc$_3$AlC is obtained from the Materials Project database [96] (material identifier mp-4079 [92]) with lattice vectors $a = 4.512\,\text{Å}$ ($a = 4.512\,\text{Å}$ and $c = 4.212\,\text{Å}$ after strain). We construct Wannier functions using WANNIER90 [97] resulting in a Wannier tight-binding model with $s$, $p$, $d$ orbitals of Sc and $s$, $p$ orbitals of Al and C. We process disentanglement with a frozen window from $-20$ to $4$ eV relative to $E_F$ but do not perform maximum localization [98]. The hoppings of the Wannier model are symmetrized [99] in real space.

To check for conflicting NLs in the BZ, we perform additional DFT calculations on the two inequivalent mirror planes $X\Gamma Z$ and $M\Gamma Z$. The results are shown in Fig. 17(e) and we observe that the only NLs in the principal gap are the two NL segments (red) spanning between the TPs of each TPP. In particular, there are no additional NLs attached to the TPs off the HSL, confirming that the TPs are type $A$, in agreement with Table I. This allows us to define an ellipsoid [whose intersections with the two mirror planes are indicated by the black ellipses in Fig. 17(e)] enclosing the TPP on which the relevant 2SW monopole charge is defined. Using the Wannier tight-binding model and the Python package Z2PACK [100,101] we compute the Wilson-loop spectrum on the ellipsoid [cf. Fig. 17(f)], and find that it winds once, therefore indicating $w_2 = 1$.

We further proceed to study the hinge-charge jump in strained Sc$_3$AlC. First, we calculate the traces of matrix representations obtained from VASP to get the ICRs of the energy bands at HSPs in the first BZ with the help of irrvsp [102]. The corepresentations at HSLs are then inferred using compatibility relations obtained from the Bilbao crystallographic server (BCS) [103–106]. The ICRs of the bands forming the TPP are found to be $(E; B_1, B_2)$ [cf. Fig. 17(e)]. Based on Table II, the knowledge of the rotational symmetry $C_4$, the HSL $\Gamma Z$, and the ICRs of the little cogroup of that line allows us to predict the fractional part of the hinge-charge jump $\Delta Q_{\gamma}$ to be $+\frac{1}{2}$.

To compute the hinge-charge jump explicitly and to verify the above prediction, we use the Python package PYTHTB to construct a nanowire with a $C_2$-symmetric cross section of $9.5 \times 9.5$ unit cells from the bulk Wannier tight-binding model [see Fig. 18(a)]. Recall that the placement of the ionic charge in the unit cell does not influence the hinge-charge jump. Therefore, we choose it such that it simplifies our calculations: we assume all ionic charge of a unit cell to be concentrated at WP $1b$ (at the corner of the 2D projection of the unit cell), which is also the location of the center of the cross section [cf. Fig. 18(a)]. The band structure of the nanowire is shown in Fig. 18(b) as a function of the remaining momentum $k$. Each state $\psi$ is colored according to the inverse participation ratio $\sum_i |\psi_i|^2$ where $p_i(\psi)$ is the probability of finding an electron in state $\psi$ at site $i$ in the 2D cross section. Together with the gray overlay of the bulk states, we can easily identify the in-gap surface (green) and hinge (red) states.

We now select two $k_z$ values at which the principal gap is open in the spectrum of the nanowire [yellow diamond and purple triangle in Fig. 18(b)]. Assuming that all states below the indicated gap are occupied, we compute the total charge distribution in the nanowire. The results for $k_z = 0.08$ and $0.34$, after coarse graining over a unit cell (see Appendix D1), are shown in Figs. 18(d) and 18(e), respectively. Integrating over successively larger square regions at one of the corners [cf. gray squares in Figs. 18(d) and 18(e)], we observe that the corner charge (corresponding to the hinge charge of the 3D model at the selected value of $k_z$) converges to $\frac{1}{2}$ and $0$ for $k_z = 0.08$ and $0.34$, respectively. This verifies that the jump is $\Delta Q_{\gamma} = \frac{1}{2}$, as predicted. The localization of the charge at the corners is already visible in Figs. 18(d) and 18(e) and the edge charge (corresponding to the surface charge of the 3D model) is clearly vanishing; however, there are strong oscillations of the charge on the edges. These oscillations are due to trivial surface states, as is revealed by computing the charge distribution on a slab (data not shown). Using the information about the charge distribution on the slab, we remove (see Appendix D2) this edge signal and reveal the strong localization of the net charge on the corners [cf. Figs. 18(f) and 18(g)]. Note that this removal of the charge oscillations is performed in a charge-neutral way, i.e., by changing neither the corner nor the edge charge.

**B. Nontrivial Euler monopole charge in Li$_2$NaN**

We now turn our attention to Li$_2$NaN. Reference [60] identified the compound Li$_2$NaN as an ideal candidate to observe the conversion of TPs to multiband nodal links, and developed its description using an effective four-band model which we assume in the following discussion. The compound exhibits a single pair of inversion-related TPs and no additional NLs close to the central NL (along the reciprocal lattice vector $G_3 \parallel k_z$) and TPs, as shown in Fig. 19(a). Therefore, this is also an ideal candidate for a TP-induced Euler monopole charge. The Berry phases of each band of the 3D model at the selected value of $k_z$ converges to $\frac{1}{2}$ and $0$ for $k_z = 0.08$ and $0.34$, respectively. This verifies that the jump is $\Delta Q_{\gamma} = \frac{1}{2}$, as predicted.

The localization of the charge at the corners is already visible in Figs. 18(d) and 18(e) and the edge charge (corresponding to the surface charge of the 3D model) is clearly vanishing; however, there are strong oscillations of the charge on the edges. These oscillations are due to trivial surface states, as is revealed by computing the charge distribution on a slab (data not shown). Using the information about the charge distribution on the slab, we remove (see Appendix D2) this edge signal and reveal the strong localization of the net charge on the corners [cf. Figs. 18(f) and 18(g)]. Note that this removal of the charge oscillations is performed in a charge-neutral way, i.e., by changing neither the corner nor the edge charge.

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FIG. 18. Hinge-charge jump observed in the nanowire geometry of Sc$_3$AlC. (a) Cross section of the nanowire geometry (extended along the $z$ direction) with $9.5 \times 9.5$ unit cells. The unit cells are shown as blue shaded squares, and the boundary of the nanowire indicated with a black frame. Two-dimensional Wyckoff positions (WPs) are shown as green, red, and orange points with their labels in the inset that shows an enlarged single unit cell. The scandium atoms project onto WPs 1b and 2c, the aluminum atoms onto 1a, and the carbon atoms onto 1b. Note the $C_4$ symmetry of the cross section with the center at WP 1b. The black circle in the enlarged unit cell denotes the location of the ionic charge of 8|e| per unit cell. (b) Band structure of the nanowire (colored lines) with cross section shown in (a) as a function of momentum ($k_z$) in the hinge Brillouin zone. The projected bulk bands (transparent gray) are overlaid on the nanowire spectrum. The coloring of the bands (see legend) encodes the inverse participation ratio, with a larger value indicating localization on fewer sites. Consequently, hinge-localized states are colored red, surface-localized states green, and bulk states blue. The two energy gaps to the left and to the right of the studied triple-point pair are marked by a yellow square ($k_z = 0.08$) and by a purple triangle ($k_z = 0.34$), respectively. (c) Integrated corner charge (corresponding to the hinge at the selected values of $k_z$) for the two $k_z$ cuts with filling as indicated in (b) as a function of the side length $a$ of the square integration region [cf. gray squares in (d) and (e)]. The corner charge for $k_z = 0.08$ converges to $e$ and for $k_z = 0.34$ to 0 (yellow vs purple solid lines). (d), (e) Charge distribution coarse grained over one unit cell for $k_z = 0.08$ and 0.34, respectively. The magnitude of the charge (in units of $e$) is shown by both the area of the circles as well as the color (see legend on the right). (f), (g) Charge distribution for the same values of $k_z$ after removing the contributions from the edge based on slab calculations (cf. Appendix D2). In (f) the localization of a nonzero charge on the corners is clearly visible.

as shown in Fig. 19(a), using three independent methods: (i) via the linking numbers obtained when applying strain to get proper linked nodal rings, (ii) via Wilson-loop spectra, and (iii) directly via the Euler curvature [73].

We first discuss the red NL segment. Following the argument of Sec. III, we reduce the $C_6$ rotational symmetry of Li$_2$NaN down to $C_2$ by applying tensile strain of approximately 5% in $y$ direction. This turns the NL segment into linked red and blue NL rings [cf. Fig. 19(b)]. The Berry phases $\phi_{3,4}$ of the bands forming the blue NL (i.e., bands 3 and 4) on the green contour satisfy $\phi_3 + \phi_4 = \pi$ mod $2\pi$. Thus, according to Sec. III B, the red nodal ring and consequently also the red NL segment in Fig. 19(a) carry Euler monopole charge $|\chi| = 2$. We arrive at the same conclusion based on the Wilson-loop spectrum computed on the purple ellipsoid shown in Fig. 19(a). The double winding implies [68] $|\chi| = 2$.

To verify this prediction independently, recall that the Euler class can be brought [69,107] to a form analogous to the Chern number, i.e., an integral of a curvature over the base manifold. By adopting a Hilbert-space basis for which $PT$ is represented by complex conjugation [73], the eigenstates can be gauged to be purely real. For two real Bloch bands $|u_1(k)\rangle$ and $|u_2(k)\rangle$ (which could possibly be degenerate with each other, but which must be separated by energy gaps from all other bands) one then defines the Euler curvature

$$F(k) = (\nabla_k u_1(k)) \times (\nabla_k u_2(k)),$$

i.e., as the off-diagonal component of the two-band non-Abelian Berry-Wilczek-Zee connection [69,73]. Integrating the curvature over a closed surface $S^2$ gives the Euler class

$$\chi = \frac{1}{2\pi} \int_{S^2} dS \cdot F(k) \in \mathbb{Z}.$$  

Note that the Euler class is independent of the parametrization of $S^2$, such that we can parametrize the relevant ellipsoid by...
FIG. 19. Verification of the Euler monopole charge $|\chi| = 2$ ($\chi = 0$) on the red (blue) nodal-line segment in Li$_2$NaN, based on the four-band tight-binding model of Ref. [60]. (a)–(d) Show illustrations and data for the red nodal-line segment (centered at $A$) and (e)–(h) for the blue segment (centered at $\Gamma$). (a), (e) Nodal line and triple-point configuration in the first one-and-a-half Brillouin zones $A\gamma_1$. Nodal lines in the second and third band gaps are shown in red and blue, respectively; triple points are shown in yellow. The purple ellipsoid defines the surface on which we compute the Euler class. (b), (f) Linking structure of the corresponding nodal chain configuration after applying approximately 5% tensile strain in $y$ direction. The green line shows the closed contour on which the Berry phases are computed. (c), (g) Spectrum of the Wilson-loop operators $W_{ij}(\theta)$ of bands $i$ and $j$ as indicated in the axis labels of constant latitude contours on the purple ellipsoid in (a) and (e), respectively, parametrized by the latitude angle $\theta$. (d), (h) Euler curvature $F(\theta, \phi)$ on the purple ellipsoid in (a) and (e), respectively, calculated using the algorithm from Ref. [73]. The curvature integrates to $|\chi| = 2i \int_{d}^{nt} d\theta \chi = 0i \int_{h}^{nt}$. The spherical coordinates $(\theta, \phi) \in [0, \pi] \times [0, 2\pi]$ and define

$$F(\theta, \phi) = \langle \nabla_{(\theta, \phi)} u_1(\theta, \phi) \rangle \times \langle \nabla_{(\theta, \phi)} u_2(\theta, \phi) \rangle.$$  

(17)

We utilize the algorithm of Ref. [73] implemented in Mathematica to compute the Euler curvature on the ellipsoid shown in Fig. 19(a). The resulting $F(\theta, \phi)$ is plotted in Fig. 19(d). Integration over the full ellipsoid confirms that $|\chi| = 2$.

The nontrivial value of $\chi$ implies a topological obstruction as discussed in Sec. III B: the red NL segment cannot be removed completely as long as $P\Gamma T$ symmetry is preserved. We verify this explicitly in the context of the tight-binding model of Ref. [60]. The 1D ICR involved in the TP has most of its weight on the nitrogen $\pi_z$ orbital, such that we can move the TPs towards the $A$ point by reducing the onsite energy of that orbital. We denote the change in energy by $\Delta\delta_{\text{np}} = -\delta$ eV < 0. As shown in Fig. 20, increasing $\delta$ shrinks the red NL segment until the two TPs collide at $A$. At that stage, the band degeneracy in the red energy gap has reduced to a single touching point at $A$. However, the Euler monopole charge prevents opening of the energy gap; indeed, increasing $\delta$ even further results in a conversion of the red TP segment into a nodal ring in the horizontal $k_z = \pi$ plane. Crucially, the Euler monopole charge persists in $P\Gamma T$-symmetric systems even if the horizontal $m_z$ symmetry was removed from the model.

FIG. 20. Demonstration of the topological obstruction of the red nodal-line segment in Li$_2$NaN due to the nontrivial Euler monopole charge. The nodal lines (obtained from the tight-binding model in Ref. [60]) near the rotation axis $A\Gamma\Gamma$ spanning over one-and-a-half Brillouin zones are shown, with nodes in the second and third band gaps shown in red and blue, respectively. The two triple points (yellow) can be forced to collide as described in the text by tuning a parameter $\delta$ of the tight-binding model. The triple points collide at $\delta = -8.6$, at which point the red NL segment has been reduced to only a single touching point at $A$. Increasing $\delta$ even further, a horizontal red nodal ring forms in the $ALH$ plane.
We remark that the critical three-band touching obtained by colliding the two TPs at the A point shares certain similarities with the very recently discussed Euler topology of topological acoustic triple points by Ref. [108]. The notable difference is that in our case the Euler-point degeneracy requires fine tuning of the model parameters, whereas Ref. [108] finds this to be a generic feature of the acoustic phonon branches.

Finally, we also comment on the blue NL segment. We can use the same three arguments to show that $\chi = 0$ in this case. For the argument via the linking, the relevant change is that now we need to consider bands 2 and 3, whose Berry phases along the green contour [cf. Fig. 19(f)] are both vanishing. Therefore, $\chi = 0$ despite the linking of the rings (see Sec. IIIIB and Appendix E). We arrive at the same conclusion by observing that the Wilson-loop spectrum in Fig. 19(g) does not wind. Finally, in Fig. 19(h), we present the Euler curvature for the purple ellipsoid shown in Fig. 19(e). The Euler curvature turns out to be antisymmetric with respect to reflection at $\theta = \pi/2$, such that integrating over the whole ellipsoid results again in $\chi = 0$.

VII. EXTENSION TO NONSYMMORPHIC SPACE GROUPS

Up to now, we have simplified the presented analysis by excluding nonsymmorphic SGs, i.e., SGs containing symmetries like screw rotations and glide planes. In this section we discuss these excluded cases, arguing that the inclusion of nonsymmorphic elements in the space group does not change the bulk-hinge correspondence. In particular, we reveal that Table II applies to triple-point pairs in nonsymmorphic SGs as well, with the only differences being that (i) the first row of the table “$C_n$” should be interpreted as only the point-group part of the possibly present nonsymmorphic screw symmetry (i.e., without the translation), and (ii) the mapping of ICRs of the little group to the ICRs of the little cogroup should be performed as described in Ref. [59].

To motivate the advertised result, note that our parallel work [59] shows that nonsymmorphic symmetries do not alter the classification of TPs. More precisely, as long as the HSL supports TPs (i.e., both 1D and 2D ICRs of the little group exist; due to nonsymmorphicity this property may be lost for certain HSLs on the BZ boundary), the symmetry constraints on the Bloch Hamiltonian $\mathcal{H}(k)$ due to some corepresentation of the little group $G^k$ of the HSL supporting TPs, are equivalent [59] to the constraints due to a corresponding corepresentation of the little cogroup $G^{\ell}$ (which consists of the corresponding point-group symmetries, i.e., without the translation). However, although nonsymmorphic symmetries have trivial implications for the TP classification, they may nontrivially affect the rotation eigenvalues that enter the symmetry-indicator formulas for the fractional corner and hinge charges (in particular if the rotational symmetry is replaced by a screw rotation).

Here, we argue in two steps that even in the case of a screw rotation, there is no change to the bulk-hinge correspondence derived in Sec. IV.C. First, we discuss in Sec. VIIA how to apply the symmetry-indicator formulas for corner charges in $C_n$-symmetric 2D systems [28,30] to compute momentum-resolved hinge charges in a wire geometry of 3D crystals with a screw rotation (instead of pure rotation) symmetry. Along the way, we derive that the symmetry-indicator formulas for corner charges [without assuming time-reversal symmetry (cf. Appendix A 1)] are symmetric under cyclic permutation of the rotation eigenvalues. Next, we consider in Sec. VII B the mapping of ICRs between the little group and the little cogroup of the HSL on which the TPs lie. We show that this mapping is compatible with the application of the symmetry-indicator formulas for the hinge charge, allowing us to establish the generalization of the bulk-hinge correspondence to TPs protected by a screw symmetry.

A. Fractional hinge charges due to screw rotational symmetry

Consider any SG with a nonsymmorphic rotational symmetry around the $z$ axis, $\{C_n|w\}$, where $n = 2, 3, 4, 6$ and $w$ is the nonsymmorphic translation. Note that the $x$, $y$ components of $w$, i.e., the ones perpendicular to the rotation axis, can be removed by shifting the rotation axis (this may potentially result in a change of the fractional translations associated with other symmetry elements in the SG, but this is not relevant for our argument). We end up with the screw symmetry $S_n = \{C_n|w_0, e_\ell\}$ with $m \in \mathbb{Z}$ that together with the translations $\ell \in \mathbb{Z}$ by lattice vectors generate a subgroup $G$ of the full SG (i.e., we drop the potentially present time-reversal symmetry as well as all point-group operations that are not generated by $C_n$).

Let $D$ be the representation of $G$ in which the eigenfunctions of the Hamiltonian transform and $D_k$ its restriction to the $k$ sector, i.e., a representation of the little group $G^k$. Then, for any $[R|v] \in G$,

\[ D_k([R|v])\mathcal{H}([R^{-1}|k])D_k([R|v])^{-1} = \mathcal{H}(k). \]  

(18)

In analogy with Sec. IV C, we take a 2D cut at fixed $k_z$ and define the 2D Hamiltonian $\mathcal{H}_k(k_z, k_y) = \mathcal{H}(k)$, which still satisfies Eq. (18) at any $k_{2D} = (k_z, k_y)$ and for any $[R|v] \in G$. In particular, for any 2D HSP $\Pi$ invariant under $S_n^\ell$ for some power $\ell$ of the screw symmetry, where $0 < \ell < n$ is a divisor of $n$, $\mathcal{H}_k$ commutes with the operator $D_k(S_n^\ell)$ which admits eigenvalues

\[ s^{\ell/n}_p = e^{i\frac{\pi}{\ell}(-mk_\ell + 2\pi p - 1)}, \quad p = 1, 2, \ldots, n/\ell. \]  

(19)

The above follows because $D_k(S_n^\ell)$ is a representation and $(S_n^\ell)^{\ell/n} = S_n^n = \{I|m_{\ell e_\ell}\}$, where $m_{\ell e_\ell} \in \mathbb{Z}$ is a lattice translation and therefore $D_k(\{I|m_{\ell e_\ell}\}) = e^{-im_\ell}1$, which has eigenvalues $e^{-im_\ell}$; thus, eigenvalues of $D_k(S_n^\ell)$ are $(n/\ell)^{th}$ roots of $e^{-im_\ell}$.

Next, we define the operator

\[ D_{k_{2D}}(C_n) = e^{i\frac{\pi}{n}(mk_z + 2\pi p')}D_k(S_n), \]  

(20)

which is a symmetry of the 2D Hamiltonian for any $p' \in \mathbb{Z}$:

\[ D_{k_{2D}}(C_n)\mathcal{H}_k(C_n^{-1}k_{2D})D_{k_{2D}}(C_n)^{-1} = \mathcal{H}_k(k_{2D}). \]  

(21)

We observe that $D_{k_{2D}}(C_n)$ [together with $D_{k_{2D}}(\{I|\ell t_{2D}\}) = D_k(\{I|\ell t_{2D}\})$] furnishes a representation of the 2D space group $pn$ (i.e., the 2D symmetry group generated by $C_n$ rotation with respect to a point and by translations). This implies that the Hamiltonian $\mathcal{H}_k$ describes a 2D system with $C_n$ symmetry, and that the rotation eigenvalues of its energy bands at a $C_n/\ell$-invariant HSP $\Pi$ are

\[ r^{\ell/n}_{p,p'} = e^{2\pi i \frac{p+m'\ell}{n\ell}}, \]  

(22)
where we recognize $e^{2\pi i n\ell/p}$ as defined in Eq. (2). With these eigenvalues, the symmetry-indicator formulas for the corner charge in 2D systems with rotational symmetry $C_2$, $C_3$, $C_4$, and $C_6$ [28,30], e.g., (A1)–(A3), can be directly applied to compute the fractional hinge charges even for nonsymmetric 3D SGs.

Note that a nontrivial symmetry of the formulas for the corner charges can now be easily deduced. Namely, the nonuniqueness of Eq. (20) due to the freedom of choosing $p' \in \mathbb{Z}$ implies that the symmetry-indicator formulas for the corner charges must be symmetric under cyclic permutations of the rotation eigenvalues (which correspond to the replacement $p' \mapsto p' + 1$). In particular, this applies irrespective of the nonsymmetricity, as can be seen by setting $m = 0$ in the symmetry $S_p$ above. We are not aware whether this symmetry has been previously pointed out, but it is easily verified explicitly for the symmetry class A (i.e., without time-reversal symmetry), which we checked using the generating Wannier configurations discussed in Appendix A of Ref. [30]. Time-reversal symmetry implies that the number of bands with rotation eigenvalues $\Pi_p^{(n)}$ and $(\Pi_p^{(n/1)})^*$ must match; however, this matching will generically be lost after performing a cyclic permutation of rotation eigenvalues. For this reason, the symmetry-indicator formulas derived under the assumption that time-reversal symmetry is present, i.e., Eqs. (A4) and (A5), do not manifest the symmetry under cyclic permutations of the rotation eigenvalues. If $n$ is even, a reduced symmetry of the symmetry-indicator formulas under $p' \mapsto p' + 1/2$ remains.

In summary, we have shown that the fractional hinge charges of nonsymmetric crystals in wire geometry with screw symmetry $C_{p} \{\pi/\ell, \pi\}$ are characterized by the same symmetry-indicator formulas that apply for corner charges in 2D systems with rotational symmetry $C_{6}$, after the $k_\ell$ dependence of the screw charges is removed. It remains to be shown that this removal is compatible with the identification of ICRs of the little group with those of the little cogroup described in Ref. [59]. This task is left for Sec. VII B.

### VIII. TRIPLE POINTS IN SPINFUL BAND STRUCTURES

The characterization of TPs reproduced in Table I is phrased in terms of ICRs of the little group $\mathcal{G}_k^h$ of the HSL on which the TPs lie, even though the symmetry constraints on the nodal-line structure near the TPs involve the ICRs of the little group $\mathcal{G}_k^h$. For symmetric SGs, this is explained by the fact that the ICRs of $\mathcal{G}_k^h$ restricted to elements $R \in \mathcal{G}_k^h$ (forming a group isomorphic to $\mathcal{G}_k^h$) are identical to the ones of $\mathcal{G}_k^h$: the ICR $\zeta$ of $\mathcal{G}_k^h$ is injectively mapped to the ICR $\rho$ of $\mathcal{G}_k^h$ by

\[ \forall \{R[0]\} \in \mathcal{G}_k^h: \rho(R) = \zeta(R[0]). \tag{23} \]

For nonsymmetric SGs, on the other hand, this is not the case. Nevertheless, we have shown in Ref. [59] that for little groups that support TPs a different mapping between ICRs $\zeta$ of $\mathcal{G}_k^h$ restricted to $\mathcal{G}_k^h$ and ICRs $\rho$ of $\mathcal{G}_k^h$ exists (see Appendix A in Ref. [59]): Let $\zeta^{1D}$ be any 1D ICR of $\mathcal{G}_k^h$ (e.g., the one that facilitates the formation of the discussed TP), then the ICR $\zeta$ of $\mathcal{G}_k^h$ is injectively mapped to the ICR $\rho$ of $\mathcal{G}_k^h$ by

\[ \forall \{R[\nu]\} \in \mathcal{G}_k^h: \rho(R) = \zeta^{1D}(\langle R[\nu]\rangle)^{-1}\zeta(\langle R[\nu]\rangle). \tag{24} \]

Note that, in contrast to the symmorphic case, the restriction of $\zeta$ to $\mathcal{G}_k^h$ is not a representation of $\mathcal{G}_k^h$ but a projective representation.

Here, we are interested in the rotation eigenvalues at HSLs, i.e., the eigenvalues of $\rho(C_{p\ell})$ at momenta invariant under $C_{p\ell}$ symmetry. It follows from Eq. (24) that the eigenvalues $\zeta^{1D}(\langle R[\nu]\rangle)$ and $\rho(R)$ of $\rho(C_{p\ell})$ are related as

\[ \rho(R) = \rho^{1D}(C_{p\ell})^{-1}\zeta^{1D}(\langle R[\nu]\rangle). \tag{25} \]

However, as a 1D ICR, $\rho^{1D}(C_{p\ell})$ must be one of the eigenvalues defined in Eq. (19), i.e., $\zeta^{1D}(\langle R[\nu]\rangle)$ for some $\rho \in \mathbb{Z}$. Then,

\[ \rho(R) = \zeta^{1D}(\langle R[\nu]\rangle)^{-1}\zeta^{1D}(\langle R[\nu]\rangle), \tag{26} \]

which is fully compatible with Eq. (20) for $p' = 1 - \rho$ in the sense that if $\zeta^{1D}(\langle R[\nu]\rangle)$ is one of the eigenvalues of $D_k(S_p)$, then $\rho(R)$ is the corresponding eigenvalue of $D_k^p(S_p)$. In particular, we observe that the $k_\ell$ dependence on the right-hand side of Eq. (26) cancels, and $\rho^{1D}(C_{p\ell})$ does not depend on $k_\ell$.

Given a TPF formed by four bands transforming according to certain ICRs of the little group, the relevant rotation eigenvalues used to compute the hinge-charge jump should be obtained by applying the construction described in Sec. VII A. However, the preceding paragraph implies that the same results are obtained if we first map the ICRs of the little group to ICRs of the little cogroup [cf. Eq. (24)] and then apply the symmetry-indicator formulas in (A1)–(A3) to the rotation eigenvalues obtained from the ICRs of the little cogroup. In fact, the nonuniqueness of $\rho^{1D}$ in Eq. (24) (if 1D ICRs of $\mathcal{G}_k^h$ exist) amounts precisely to the nonuniqueness of $p'$ in Eq. (20), further evincing how the two presented descriptions are two facets of the same argument. We therefore conclude that both the TP types and the hinge-charge jumps can be determined from the ICRs of the little cogroup, which implies that the bulk-hinge correspondence derived in Sec. IV C directly applies to nonsymmetric SGs as well.
distinguished in the corresponding symmetry indicators, and they all result in the same value of jumps $\Delta Q_c$ and $\Delta P$.

For simplicity, we restrict the explicit analysis to the case when the $C_3$ rotation center of the sample resides at the 1a WP (a straightforward analysis using the symmetry-indicator formulas from Ref. [30] reveals that our results remain true if the rotation center resides at WP 1b or 1c). Similar to Sec. IV, we set all ionic charge to WP 1a. Then, the corner charge on a 2D cut is given by (cf. class A in Ref. [30])

$$Q_c^{(3)} = \left( \left( K_1^{(3)} \right) + \left( K_2^{(3)} \right) + \left( K_3^{(3)} \right) \right) \mod e.$$

(27)

The square brackets are defined in the exact same way as in the spinless case, $[\Pi_p^{(n)}] = \# \Pi_p^{(n)} - \# \Pi_p^{(n)}$; however, the labeling of rotation eigenvalues in Eq. (2) is replaced by

$$\Pi_p^{(n)} = e^{2\pi i (p-1)/n} e^{i \pi /n}, \quad p = 1, 2, \ldots, n.$$

(28)

The bulk polarization can similarly be expressed in terms of the symmetry indicators as [29,30]

$$P^{(3)} = \left( \frac{e}{3} \left( 2 \left( K_1^{(3)} \right) + \left( K_2^{(3)} \right) + \left( K_3^{(3)} \right) \right) \mod e R. \right.$$

$$+ 2 \left( \left( K_2^{(3)} \right) \right) \mod e R.$$  

(29)

By performing an analysis (not appended) similar to the one detailed in Appendixes A3 and A4 for the spinless case, we derive the bulk-hinge correspondence for spinful TPPs in triangular geometry. Independent of the HSL on which the TPP lies and regardless of the WP of the rotation center, the hinge-charge jump is universally found to be

$$\Delta Q_c = \frac{e}{3} \mod e.$$

(30)

and the jump of the bulk polarization

$$\Delta P = 0 \mod e R.$$  

(31)

We observe that even in spinful systems, all TPPs carry fractional hinge-charge jump.

The derived results directly apply to TPPs reported in WC-type crystalline materials reported by Ref. [49]. In particular, TaN exhibits a type-($A$, $A$) TPP characterized by a hinge-charge jump $\frac{e}{3}$ along the $GA$ line. Furthermore, this material is very close to the ideal semimetallic TPP case, with only small additional Fermi pockets around the $K$ point and $A$ point of the BZ. We have considered extracting the predicted hinge-charge jump for TaN from first-principles calculations (as we have done for Sc$_2$AIC under strain), however, the absence of a surface gap has prevented us from doing so. In the future, a systematic check of the materials that host TPPs for open surface gaps could lead to a better material candidate.

**IX. CONCLUSIONS AND OUTLOOKS**

In this work we exposed higher-order topological fingerprints of triple nodal points (TPPs) in three dimensions (3D). Our focus has been on the spinless case, where one encounters an interplay of band nodes with a rich topological structure: nodal lines (NLs) can be protected by mirror ($m_n$) planes, NLs governed by non-Abelian topology and equipped with monopole charges can be stabilized by space-time inversion ($PT$) symmetry, and either species of NLs can be pinned to high-symmetry lines (HSLs) by rotation ($C_n$) or antunitary rotation ($C_nPT$) symmetry. In particular, triple-point pairs (TPPs; formed when a 2D irreducible corepresentation (ICR) crosses a pair of 1D ICRs) are semimetallic features where a NL along a HSL is transferred across three adjacent energy gaps.

The rich topological structure of spinless systems supporting TPPs prompted us to analyze HSLs with 13 distinct magnetic little cogroups, summarized by Table I. The main finding of our analysis is that triple-point pairs demarcated by a pair of type-$A$ or by a pair of type-$B$ TPPs are generally characterized by a fractional jump of the hinge charge. These results apply also to nonsymmorphic space groups. On top of the spinless analysis, in the last section we briefly considered the spinful case, where TPPs arise in the presence of $C_{3v}$ symmetry, and where a fractional hinge-charge jump is also predicted to be a universal higher-order feature of TPPs. Note that while three-dimensional Weyl nodes and Dirac nodes exist in both the higher-order [40–47] and first-order [87,109] varieties, we report that all type-($A$, $A$) and type-($B$, $B$) TPPs are universally associated with the higher-order bulk-hinge correspondence. Our finding thus overcomes the previous unsuccessful search for a general bulk-boundary characterization of TPPs in surface states [49,52,57,61], as conventionally associated with first-order topology.

Although our analysis in the presence of $C_4$ rotational symmetry explicitly assumed a primitive tetragonal Bravais lattice, the result in Table II generalizes with no alterations to the body-centered tetragonal case. To understand this, note that the derivation of the hinge-charge jump (cf. Appendix A 3b) is based on considering a two-dimensional (2D) system with $C_n$ symmetry. It is found that (1) the ICRs at the $\Gamma$ and at the $M$ point of the 2D square lattice are identical, and that (2) the corner-charge jump associated with a band inversion of a 2D ICR with two 1D ICRs is also identical for both the $\Gamma$ and at the $M$ point. The 3D models with tetragonal (either primitive or body-centered) symmetry are obtained from the 2D systems by interpreting the band-inversion-tuning parameter as a third momentum component $k_z$. The difference between the two Bravais lattices merely corresponds to the way the periodically changing Hamiltonians $\mathcal{H}_t(k_{2D}) = \mathcal{H}_{t, k_{2D}}(k_{2D})$ are glued together: for the body-centered case, $\mathcal{H}_t(k_{2D}) = \mathcal{H}_{t, +\frac{\pi}{2}}(k_{2D} + \Gamma - M)$, whereas such a constraint is absent for the primitive case. It is clear that the mathematical analysis of the hinge-charge jump in Sec. IV C leading to Table II applies irrespective of this additional constraint. An analogous argument in the presence of $C_3$ also reveals why in the trigonal case we find identical classification of TPPs along the lines $\Gamma$, $K$, and $K'$. 

While the presented spinless material Sc$_2$AIC [57] requires unrealistic values of applied strain to realize the quantized hinge-charge jump, our analysis demonstrates that the discussed phenomenology could conceivably be realized and observed in crystalline solids if more appropriate compounds are identified in the future. Furthermore, metamaterial realizations (e.g., in acoustics, similar to those of Refs. [42,47]) are definitely feasible.

Finally, it is interesting to speculate whether a similar universal higher-order bulk-boundary correspondence extends to other previously reported one-dimensional nodal structures;
for example, aside from the nodal-line segment spanned by a TPP which has been considered by this work, nodal-line chains [66,90,110], gyroscopes [35,111,112], and starfruits [113] were proposed. They all require crossing of bands with particular choices of symmetry eigenvalues which is associated with a change of the symmetry indicators, potentially implying similar phenomenology of higher-order topological hinge-charge jumps. Given the numerous material candidates for the various nodal-line compositions, it should be of theoretical as well as of experimental interest to consider such generalizations in the future.

We provide access to all the data and code necessary to reproduce the results presented here in the supplementary data and code [114].

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APPENDIX A: CORNER AND HINGE CHARGES

In this Appendix we derive various statements presented in Sec. IV in relation to the second Stiefel-Whitney (2SW) class and hinge charges. For reference, we include the relevant symmetry-indicator formulas for the corner charge of spinless 2D systems with $C_n$ symmetry [28,30], including both the case without (with) spinless time-reversal symmetry, in Appendix A.1. Next, in Appendix A.2 we show that in spinless 2D systems with $C_2T$ and $C_n$ symmetries, where $n = 4, 6$, the 2SW class can be written in terms of $C_4$ and $C_6$ symmetry indicators. In particular, we prove Eq. (6) from Sec. IV.A. Then, in Appendix A.3 we consider triple-point pairs (TPPs), i.e., pairs of triple points (TPs) formed by consecutive triplets of bands, protected by $C_n$ symmetry, where $n = 3, 4, 6$, in spinless systems with $\mathcal{P}T$ symmetry. We derive Table II presented in Sec. IV C which gives the jumps in the 2SW class of 2D cuts and in the hinge charge for the different combinations of irreducible corepresentations. Finally, in Appendix A.4 we discuss why TPPs are not associated with a jump in the surface charge.

1. Symmetry-indicator formulas for the corner charge

Here we list the symmetry-indicator formulas for the corner charges $Q_{\text{c},\text{la}}^{(n)}$ of 2D crystals with $C_n$ symmetry in the corresponding geometries shown in Fig. 7(a) with the center of the sample located at the Wyckoff position (WP) $mX$ (cf. Ref. [30] for the labeling of WPs). In all cases we assume that the ionic charges are placed at WP la and we use the notation of Ref. [28], defined in Eqs. (2) and (3), for the labeling of rotation eigenvalues and symmetry indicators.

In the absence of time-reversal symmetry (symmetry class $A$), Ref. [30] derives the formulas to be the following: for $n = 3$,

\[
Q_{\text{c},\text{la}}^{(3)} = \frac{e}{3} \left( [K_1^{(3)}] + [K_2^{(3)}] + [K_3^{(3)}] \right) \mod e, \tag{A1a}
\]

\[
Q_{\text{c},ib}^{(3)} = -\frac{e}{3} \left( [K_1^{(3)}] + [K_2^{(3)}] \right) \mod e, \tag{A1b}
\]

\[
Q_{\text{c},lc}^{(3)} = -\frac{e}{3} \left( [K_2^{(3)}] + [K_1^{(3)}] \right) \mod e; \tag{A1c}
\]

for $n = 4$,

\[
Q_{\text{c},la}^{(4)} = \frac{e}{4} \left( -[X_1^{(2)}] + \frac{1}{2}M_1^{(4)} - \frac{3}{2}M_3^{(4)} \right) \mod e, \tag{A2a}
\]

\[
Q_{\text{c},lb}^{(4)} = \frac{e}{4} \left( X_1^{(2)} - \frac{3}{2}M_1^{(4)} + \frac{1}{2}M_3^{(4)} \right) \mod e; \tag{A2b}
\]

and for $n = 6$,

\[
Q_{\text{c},la}^{(6)} = -\frac{e}{6} \left( 2[K_1^{(3)}] + \frac{3}{2}M_1^{(2)} \right). \tag{A3}
\]

If spinless time-reversal symmetry $\mathcal{T}$ satisfying $\mathcal{T}^2 = +\mathbb{I}$ is present, i.e., in symmetry class $A\mathbb{I}$, the formulas simplify due to constraints on the topological invariants $[\Pi^p_{\text{d}}]^{(n)}$ [30]. In our work, this case only occurs for $n = 4$,

\[
Q_{\text{c},la}^{(4)} = \frac{e}{4} \left( -[X_1^{(2)}] + 2M_1^{(4)} + 3M_2^{(4)} \right) \mod e, \tag{A4a}
\]

\[
Q_{\text{c},lb}^{(4)} = \frac{e}{4} \left( [X_1^{(2)}] + 2M_1^{(4)} + 3M_2^{(4)} \right) \mod e, \tag{A4b}
\]

and for $n = 6$,

\[
Q_{\text{c},la}^{(6)} = \frac{e}{4} M_1^{(4)} + \frac{e}{6} K_1^{(3)} \mod e. \tag{A5}
\]

Finally, we also need the formula for $n = 2$, which is given in Ref. [28]:

\[
Q_{\text{c},la}^{(2)} = \frac{e}{4} \left( -[X_1^{(2)}] - [X_2^{(2)}] + M_1^{(2)} \right) \mod e. \tag{A6}
\]

2. Stiefel-Whitney insulators with rotational symmetry

a. $C_4$ symmetry

We first consider $C_4$ symmetry. The four time-reversal-invariant momenta are $\Gamma, X, X', M$, where $X, X'$ are equivalent. According to Eq. (5) a nontrivial 2SW class is equivalent to

\[
\left[ \frac{1}{2} \# \Gamma_1^{(2)} \right] + 2 \left[ \frac{1}{2} \# X_2^{(2)} \right] + \left[ \frac{1}{2} \# M_1^{(2)} \right] = 1 \mod 2. \tag{A7}
\]

This does not constrain $\# X_2^{(2)}$ at all, but it is equivalent to either

\[
\left[ \frac{1}{2} \# \Gamma_1^{(2)} \right] = 0 \mod 2 \wedge \left[ \frac{1}{2} \# M_2^{(2)} \right] = 1 \mod 2 \nonumber
\]

\[
\Leftrightarrow \quad \# \Gamma_1^{(2)} \in \{0, 1\} \mod 4 \wedge \# M_2^{(2)} \in \{2, 3\} \mod 4 \nonumber
\]

\[
\Rightarrow \quad \# M_2^{(2)} - \# \Gamma_1^{(2)} = : \left[ M_2^{(2)} \right] \in \{1, 2, 3\} \mod 4 \nonumber
\]

or the same with $\Gamma$ and $M$ exchanged, where the latter implies $\left[ M_2^{(2)} \right] \in \{1, 2, 3\} \mod 4$ as well. Thus, $w_2 = 1$ implies
\[ [M_2^{(2)}] \in \{1, 2, 3\} \pmod{4}. \]

On the other hand, \( w_2 = 0 \) implies

\[ \left\lfloor \frac{1}{3} \right\rfloor \Gamma_2^{(2)} = \left\lfloor \frac{1}{3} \right\rfloor M_2^{(2)} \pmod{2} \]

\[ \Rightarrow \left[ M_2^{(2)} \right] \in \{0, 1, 3\} \pmod{4}. \]

Furthermore, time reversal combined with \( C_4 \) symmetry imply [28] that \( [M_4^{(4)}] = [M_2^{(4)}] \), such that together with \( [M_2^{(2)}] = [M_2^{(4)}] + [M_4^{(4)}] \) (which follows from \( C_4^2 = C_2 \)) we find

\[ [M_2^{(2)}] = 2[M_2^{(4)}]. \]  \hspace{1cm} (A8)

Therefore, \( [M_2^{(2)}] \) has to be even. Since we already restricted \( [M_2^{(2)}] \) for \( w_2 = 1 \) to the set \( \{1, 2, 3\} \pmod{4} \) (and to the set \( \{0, 1, 3\} \pmod{0} \) for \( w_1 = 0 \), selecting the even element of the corresponding set results in

\[ w_2 = \frac{1}{2}[M_2^{(2)}] \pmod{0} = [M_2^{(4)}] \pmod{2}. \]  \hspace{1cm} (A9)

Finally, using Eq. (A9) and assuming vanishing bulk polarization, \( [X_1^{(2)}] = 0 \) [28], we can rewrite Eq. (A4a) as

\[ Q^{(4)} = \frac{e}{4}(2[M_4^{(4)}] + 3w_2) \pmod{e}. \]  \hspace{1cm} (A10)

We observe that for \( w_2 = 1 \) the term in the brackets is an odd integer, while it is an even integer for \( w_2 = 0 \). This restricts the fractional part of \( Q^{(4)} \) to \( \pm \frac{e}{2} \) in the first, and to \( 0 \) or \( \pm \frac{e}{2} \) in the second case.

**b. \( C_6 \) symmetry**

Next, we consider \( C_6 \) symmetry, where the four time-reversal-invariant momenta are \( \Gamma, M, M', \) and \( M'' \) with the latter three being equivalent. Correspondingly,

\[ \left\lfloor \frac{1}{3} \right\rfloor \Gamma_2^{(2)} + 3\left\lfloor \frac{1}{3} \right\rfloor M_2^{(2)} = 1 \pmod{2}. \]  \hspace{1cm} (A11)

A nontrivial value \( w_2 = 1 \) implies, in analogy with the analysis of the \( C_4 \)-symmetric case, that

\[ [M_2^{(2)}] \in \{1, 2, 3\} \pmod{4}, \]  \hspace{1cm} (A12)

while \( w_2 = 0 \) implies

\[ [M_2^{(2)}] \in \{0, 1, 3\} \pmod{4}. \]  \hspace{1cm} (A13)

For the next step in our reasoning we need to apply the following property: if \( [M_2^{(2)}] = 1 \pmod{2} \), then the bulk is necessarily gapless. This can be seen as follows. By assumption, the number of occupied bands with \( C_2 \)-rotation eigenvalue 1 changes by an odd number between \( \Gamma \) and \( M' \):

\[ \#M_1^{(2)} - \#\Gamma_1^{(2)} = [M_2^{(2)}] = 1 \pmod{2}. \]  \hspace{1cm} (A14)

Since the \( C_2 \) symmetry acts as inversion on the 1D BZ segment \( \Gamma \Delta M \Gamma \), Eq. (A14) implies [34] that the occupied bands carry a total Berry phase \( \pi \) mod 2 on that segment. We further consider the triangle formed by the \( \Gamma \Delta M \Gamma \) paths of the three BZs around a \( K \) point, as illustrated in Fig. 21. Due to the sixfold rotational symmetry the three sides of the triangle all contribute \( \pi \pmod{2\pi} \) to the Berry phase, such that the total Berry phase along the triangular contour is \( \pi \pmod{2\pi} \), indicating that there are an odd number of band nodes (formed between the occupied and the unoccupied bands) inside the triangle, i.e., the bulk is gapless. Conversely, a gapped bulk implies \( [M_2^{(2)}] = 0 \pmod{2} \). Noting that \( [M_1^{(2)}] = -[M_2^{(2)}] \)

\[ \text{(because } \sum_{n=1}^{\infty} [\Pi_{\rho}^{(n)}] = 0 \text{ [28]}, \text{ an insulating bulk structure equivalently requires } [M_2^{(2)}] \text{ to be even. Therefore,} \]

\[ w_2 = \frac{1}{2}[M_2^{(2)}] \pmod{2}. \]  \hspace{1cm} (A15)

Using Eq. (A15) (and noting that for \( C_6 \)-symmetric systems the bulk polarization always vanishes [28]), we can rewrite Eq. (4b) for the corner charge as

\[ Q^{(6)} = \frac{e}{6}\left([K_1^{(3)}] + 3w_2\right) \pmod{e}. \]  \hspace{1cm} (A16)

It follows from time-reversal symmetry that at HSPs states have either real rotation eigenvalues or come in pairs with complex-conjugate rotation eigenvalues. In particular, this implies that \( [K_2^{(3)}] = [K_3^{(3)}] \) and because of the same number of filled bands at points \( K \) and \( \Gamma \), it follows that

\[ [K_1^{(3)}] = -[K_2^{(3)}] - [K_3^{(3)}] = 0 \pmod{2}, \]  \hspace{1cm} (A17)

i.e., \( [K_n^{(3)}] \) is an even integer. Thus, the term in brackets in Eq. (A16) is an odd integer for \( w_2 = 1 \) and an even integer for \( w_2 = 0 \). This restricts \( Q^{(6)} \) to \( \pm \frac{e}{6} \) or \( 0 \) in the first case, and to \( 0 \) or \( \pm \frac{e}{6} \) in the second case.

**3. Hinge-charge jump and 2SW monopole due to triple points**

We start from the classification of TPs in spinless \( \mathcal{PT} \)-symmetric systems as presented in Ref. [60] for little cogroups \( \mathcal{G} = C_{3(h)}, C_{4(h)}, C_{6(h)} \) of some high-symmetry line (HSL) and we consider the situation depicted in Fig. 9. We compare quantities in the orange \( k_t \) range (to the left of the first TP, where the 2D ICR \( \rho_2^{3D} \) is occupied) and the blue \( k_e \) range (to the right of the second TP, where the two 1D ICRs \( \rho_a^{1D} \) and \( \rho_b^{1D} \) are occupied). For the ICRs the notation of Ref. [65] is used. In particular, when defining the changes \( \Delta Q, \Delta w, \) we subtract the first (orange \( k_t \) range) from the latter (blue \( k_e \) range). For each 2D or 1D ICR \( \rho \) of \( C_3^{(2)} \cup (\mathcal{PT})C_3^{(2)} \),

\[ \phi_{\Delta M} = \pi. \]

\[ \text{FIG. 21. Three hexagonal Brillouin zones around a } \Gamma \text{ point of a } C_6 \text{-symmetric model. Assuming } [M_2^{(2)}] = 1 \pmod{2} \text{ the total Berry phase } \phi_{\Delta M} \text{ of the occupied bands along the closed contour } \Gamma \Delta M \Delta \Gamma \text{ equals } \pi \text{ (cf. Appendix A2b). Therefore, the Berry phase along the triangular contour (green) is also } \phi_{t} = 3\pi = \pi \mod 2\pi. \text{ The result implies that the triangle encloses an odd number of band nodes in the principal gap (red disks), i.e., the system is not an insulator.} \]
we look up the corresponding rotation eigenvalues on the Bilbao crystallographic server (BCS) \[103–105\] using the program COREPRESENTATIONSPG \[82,83\] and, assuming there are no other band inversions in the principal gap, compute the relevant symmetry indicators (see Tables IV, V, and VII). Before proceeding with the mathematical analysis, we make two remarks. First, note that the HSL on which the TPs lie does not need to go through the center of the BZ (point \(\Gamma\) of the 2D cut). Namely, the little cogroup \(C_{\nu}\) is also realized at the \(K\) point(s) of space groups (SGs) with threefold or sixfold rotational symmetry, while \(C_{\nu}\) is also realized at \(M\) points of SGs with fourfold rotational symmetry.

In all cases we assume that the SG contains \(\mathcal{PT}\), acting as \((C_2T)_{2D}\) in the 2D cuts, and \(C_6\) with order \(n\) in \([3,4,6]\). Furthermore, we place all ionic charge at the center of the unit cell because, ultimately, we are interested in the change of the corner charge as a function of \(k\), and the ionic charge distribution does not depend on \(k\). If the system symmetry is \(C_3\), then \(\mathcal{T}_{2D} \equiv (C_2 PT = m_1 T)\) is not present, such that the corner charge is given by Eq. (A1). For SG symmetries with rotation of order \(n = 4, 6\), the \(C_2\) combines with \(\mathcal{PT}\) to give \(C_2 \mathcal{PT} = \mathcal{T}_{2D}\), such that we can apply the simplified formulas (A4) and (A5). For the 2SW class, we use the results of the previous subsection, i.e., Eqs. (A9) and (A15).

We next go in detail through all the possible cases.

### a. Triple points along \(C_{3(\nu)}\)-symmetric lines

For \(C_{3(\nu)}\) there is only one possible configuration of two TPs, namely, the one with ICRs \((E;A,A)\). The symmetry indicators (cf. Table IV) imply that \(\Delta \#\Pi^{(3)} = 2\) and \(\Delta \#\Pi^{(5)} = -1\).

Let us first consider TPs occurring along the HSL \(\Pi = \Gamma\) of a \(C_3\)-symmetric system. If the rotation center of the sample lies at WP 1a, then \(\Delta[K^{(3)}] = \Delta[K^{(3)}] = -\Delta \#\Pi^{(3)}\). Then, according to Eq. (A1a), the hinge-charge jump is

\[
\Delta Q^{(3)}_{\Pi,1a} = \frac{2e}{3} \left( \Delta \#\Pi^{(3)} + \Delta \#\Pi^{(5)} \right) \mod e = \frac{e}{3} \mod e. \tag{A18}
\]

If the TPs instead occur along HSL \(\Pi = K\) (or equivalently \(K^{*}\)) of a \(C_3\)-symmetric system (with rotation center still set to 1a), then \(\Delta[K^{(3)}] = \Delta \#\Pi^{(3)}\) such that

\[
\Delta Q^{(3)}_{\Pi,1a} = \frac{e}{3} \left( \Delta \#\Pi^{(3)} + \Delta \#\Pi^{(5)} \right) \mod e = \frac{e}{3} \mod e. \tag{A19}
\]

It is easily verified by using Eqs. (A1b) and (A1c) that the derived results for \(\Delta Q^{(3)}\) remain unchanged if the rotation center of the finite system is instead located at WP 1b or 1c.

If \(\Pi = K\) of a \(C_{\nu}\)-symmetric system, then we need to use Eq. (A5) instead, resulting in the same

\[
\Delta Q^{(6)}_{\Pi,1a} = \frac{e}{6} \Delta \#\Pi^{(3)} \mod e = \frac{e}{3} \mod e. \tag{A20}
\]

This concludes the derivation of \(\Delta Q^{(6)}\) for TPs along \(C_{\nu}\)-symmetric lines.

We briefly analyze the jump \(\Delta w_2\) of the 2SW class. We have argued in Sec. IV C and demonstrated in Sec. VD that the 2SW class is not symmetry indicated for \(C_3\)-symmetric systems. For \(C_6\), on the other hand, we use Eq. (A15) to find

\[
\Delta w_2 = \frac{1}{6} \Delta[M^{(2)}_{1a}] = 0, \tag{A21}
\]

because, by assumption, there is neither a band inversion at \(\Gamma\) nor at \(M\).

#### b. Triple points along \(C_{4(\nu)}\)-symmetric lines

Next, we consider \(C_{4(\nu)}\)-symmetric lines with ICRs and symmetry indicators given in Table V. Here, we need to distinguish three TP configurations (namely, \((E;A,A), (E;B,B)\), and \((E;A,B)\)) and two HSLs (namely, \(\Pi = \Gamma\) and \(\Pi = K\). The differences \(\Delta \#\Pi^{(1)}\), \(\Delta \#\Pi^{(3)}\), and \(\Delta \#\Pi^{(5)}\) for the various TP configurations are listed in Table VI. By recalling Eq. (A9), we find that for all cases

\[
\Delta w_2 = \Delta[M^{(4)}_{1a}] \mod 2 = 1 \mod 2, \tag{A22}
\]

in agreement with the fact that the TPs are type \(A\) (cf. Sec. IIIA).

To identify the jump in the hinge charge, we have to analyze the two HSLs separately. First, for \(\Pi = \Gamma\) we have \(\Delta[P^{(6)}] = -\Delta \#\Pi^{(6)}\) for both \(P \in \{K, M\}\), and the change in corner charge is given by

\[
\Delta Q^{(4)}_{\Pi,1a} = -\frac{e}{4} (\mp \Delta \#\Pi^{(2)} + 2 \Delta \#\Pi^{(4)} + 3 \Delta \#\Pi^{(6)} \mod e. \tag{A23}
\]

where the negative (positive) sign of \(\Delta \#\Pi^{(2)}\) corresponds to setting the center of the system to WP 1a (1b). Observe in Table V that \(\Delta \#\Pi^{(2)}\) is even for all TPs, which means that the “±” sign ambiguity is unimportant, and both WPs lead to the same value of the hinge-charge jump.

In contrast, for \(\Pi = M\) we obtain contributions from \(\Delta[M^{(4)}_{1a}] = \Delta \#\Pi^{(6)}\), leading to

\[
\Delta Q^{(4)}_{\Pi,1a} = \frac{e}{4} (2 \Delta \#\Pi^{(4)} + 3 \Delta \#\Pi^{(6)} \mod e. \tag{A24}
\]

Careful evaluation of Eqs. (A23), (A24), and (A32) for all combinations of ICRs gives the following results: For TPs

| ICRs for | Eigenvalues of | Symmetry indicators at \(\Pi\) |
|---------|---------------|-------------------------------|
| \(C_{4a}\) | \(C_4\) | \(C_2\) | \(C_4\) | \(\#\Pi^{(3)}\) | \(\#\Pi^{(5)}\) |
| \(A_1, A_2\) | \(A\) | 1 | 1 | 1 | 1 | 0 |
| \(B_1, B_2\) | \(B\) | 1 | -1 | 1 | 0 | 0 |
| \(E\) | \(E\) | -1, -1 | \(i, -i\) | 0 | 0 | 1 |
Each TPP is specified by the irreducible corepresentations (ICRs) \((\rho^{2D}; \rho_{u}^{1D}, \rho_{v}^{1D})\) on a fourfold rotation axis, corresponding to the high-symmetry point \(\Gamma = \Gamma\) in a 2D cut perpendicular to the rotation axis. The changes are defined by subtracting the characteristics of the systems with \(\rho^{2D}\) occupied from those of the system with \(\rho_{u,v}^{1D}\) occupied. The hinge-charge jump is computed using Eq. (A23) for \(\Pi = \Gamma\) and Eq. (A24) for \(\Pi = M\), while \(\Delta w_2\) is computed from Eq. (A9).

Along either \(\Gamma\) or \(M\), \(\Delta Q^{\text{Q}} = \frac{\pi}{4}\) for both \((E; A, A)\) and \((E; B, B)\). The results are summarized in Table VI.

c. Triple points along \(C_{6v}\)-symmetric lines

There is only one HSL with little cogroup \(C_{6v}\) (namely, \(\Gamma\) in \(C_{6v}\)-symmetric systems), and considering the possible crossings of ICRs (listed in Table VII) results in six distinct TPP configurations. We first focus on the cases where the two TPs are of the same type, which gives the four TPs listed in Table VIII. By combining \(\Delta [\Pi_1^{(p)}] = -\Delta [\Pi_1^{(p)}]\) (for \(\Pi \in \{M, K\}\)) with Eqs. (A5) and (A15), we calculate the jumps

\[
\Delta Q^{\text{Q}} = -\frac{\epsilon}{4} \Delta \Gamma^{\text{I}}_{1} - \frac{\epsilon}{6} \Delta \Gamma^{\text{I}}_{1} \text{ mod } e, \tag{A25}
\]

\[
\Delta w_2 = -\frac{1}{2} \Delta \Gamma^{\text{I}}_{1} \text{ mod } 2. \tag{A26}
\]

The computed values of \(\Delta Q^{\text{Q}}\) and of \(\Delta w_2\) for all the TPPs where both TPs are of the same type are listed in Table VIII. We find that a nontrivial change of the 2SW class, which occurs for two type-\(A\) TPs, is associated with a hinge-charge jump \(\Delta Q^{\text{Q}} = \frac{\pi}{4}\). In contrast, pairs of type-\(B\) TPs are characterized by trivial \(\Delta w_2 = 0\) and are associated with a hinge-charge jump of \(\Delta Q^{\text{Q}} = \frac{\pi}{4}\).

TABLE VII. Rotation eigenvalues and symmetry indicators for all irreducible corepresentations of \(C_{6v}\) with \(\mathcal{PT}\) at the high-symmetry point \(\Gamma\) of a \(C_{6v}\)-symmetric system. The list of ICRs is unchanged if \(\mathcal{PT}\) symmetry is removed in the case of \(C_{6v}\).

| ICRs for \(C_{6v}\) | Eigenvalues of \(C_6\) | Symmetry indicators at \(\Gamma\) |
|---------------------|---------------------|-------------------------------|
| \(C_6\) | \(C_2\) | \(C_3\) | \(\#\Gamma^{(2)}\) | \(\#\Gamma^{(3)}\) |
| \(A_1, A_2\) | \(A\) | 1 | 1 | 1 | 1 |
| \(B_1, B_2\) | \(B\) | \(-1\) | 1 | 0 | 1 |
| \(E_1\) \(2E_1 E_2\) | \(-1, -1\) | \(e^{2\pi i/3}, e^{-2\pi i/3}\) | 0 | 0 |
| \(E_2\) \(2E_1 E_2\) | \(1, 1\) | \(e^{2\pi i/3}, e^{-2\pi i/3}\) | 2 | 0 |

TABLE VIII. Changes in symmetry indicators (\(\Delta \#\Pi^{(p)}\)), hinge charge (\(\Delta Q^{\text{Q}}\)), and second Stiefel-Whitney class (\(\Delta w_2\)) associated with the different configurations of triple-point pairs (TPPs) along the \(\Gamma\) line of \(C_{6v}\)-symmetric systems. Each TPP is specified by the irreducible corepresentations (ICRs) \((\rho^{2D}; \rho_{u}^{1D}, \rho_{v}^{1D})\) along the \(\Gamma\) line. For simplicity we use the labels of ICRs for \(C_{6v}\), the corresponding notation for \(C_6\) can be extracted from Table VII. The changes are defined by subtracting the characteristics of the systems with \(\rho^{2D}\) occupied from those of the system with \(\rho_{u,v}^{1D}\) occupied. The values of \(\Delta Q^{\text{Q}}\) and \(\Delta w_2\) are computed from Eq. (A25) and (A26), respectively.

| TP types | \((E; A, A)\) | \((E; B, B)\) |
|----------|---------------|---------------|
| ICRs     | \((E_1; A_1, A_1)\) | \((E_1; B_1, B_1)\) | \((E_2; A_1, A_1)\) |
| \(\Delta \#\Gamma^{(2)}\) | 2 | -2 | 0 | 0 |
| \(\Delta \#\Gamma^{(3)}\) | 2 | 2 | 2 | 2 |
| \(\Delta Q^{\text{Q}}\) | 0 | 0 | 0 | 0 |
| \(\Delta w_2\) mod 2 | 1 | 1 | 0 | 0 |

Finally, there is the possibility to have two TPs of different types, i.e., one type \(A\) and one type \(B\), by choosing one of the following ICR combinations: \((E_1; A_1, B_1), (E_2; A_1, B_1)\). In these two cases, we find that \(\Delta [\Gamma_1^{(2)}] = -\Delta [\Gamma_1^{(2)}] = 1\) mod 2 (i.e., it is an odd number). This implies that the value of \([\Gamma_1^{(2)}]\) must be odd on one side of the TPP. However, recall from Appendix A2 that a gapped bulk requires \([\Gamma_1^{(2)}] = 0\) mod 2. It therefore follows that the bulk is necessarily gapless on one side of the TPP, such that the hinge-charge jump cannot be defined in this case. This finding is consistent with the intuitive explanation given in the main text, where the different type of the two TPs forces the attached NL arcs to cross the orange or blue \(k\) range. In Fig. 10(c), a 2D cut in the orange \(k\) range would correspond to the situation shown in Fig. 21 with the red disks corresponding to places where the red attached NL arcs cross the 2D cut.

4. No jump of the surface charge due to triple points

For the hinge-charge jump to be observable, it is important that the surface charge (more precisely, the surface charge density; this corresponds to the edge charge density of the 2D cuts at fixed \(k_z\)) is vanishing [28] for the \(k_z\) ranges on both sides of the TPP. This can only be true if the jump of the surface charge associated with the TPP is zero. Here we show that this is indeed true for all the TPPs shown in Table II.

Before deriving the desired fact mathematically from the corresponding symmetry-indicator formulas, let us present a simple argument based on the quantization of Berry phase. Namely, recall that for a boundary of a high-symmetry orientation with respect to the crystalline axes, the surface charge is in a one-to-one correspondence [81] with the Berry phase along a closed momentum-space (k) path along the direction perpendicular to the considered surface. Here, first recall [59,60] that stable TPs require the presence of either \(\mathcal{PT}\) symmetry (in which case the Berry phase is quantized to \(0 \lor \pi\) on any closed \(k\) path due to the reality condition [68]) or of \(m_n\) mirror symmetry (in which case the mirror symmetry acts like inversion on the straight \(k\) paths perpendicular to the
boundaries considered in Figs. 2, 14, and 15, thus quantizing the Berry phase of interest to 0 vs \( \pi \) [115]).

The quantization of the Berry phase implies that the surface charge can only change if the \( \pi \) the Berry phase of interest to 0 vs arbitrarily jump to be observable) at least when the boundaries are oriented symmetrically with respect to the crystal axes.

More formally, we now derive the same conclusion for an arbitrarily oriented \( C_n \)-symmetric system. In such a case the surface charge density of a gapped 2D crystal is given [80] by \( \sigma_{\text{surf}} = \mathbf{P} \cdot \mathbf{n} \), where \( \mathbf{P} \) is the bulk polarization and \( \mathbf{n} \) the surface normal. To prove that \( \Delta \sigma_{\text{surf}} = 0 \) across the TPP for arbitrary boundary termination, it needs to be true that \( \mathbf{P} \cdot \mathbf{n} = 0 \) when moving across the TPP. Similar to the corner charge, the bulk polarization \( \mathbf{P}(n) \) of a 2D crystal with \( C_n \) rotational symmetry can be expressed [28–30] using symmetry indicators. For \( C_3 \)-symmetric crystals, we use the result of Refs. [29,30] which does not assume time-reversal symmetry to be present,

\[
\mathbf{P}^{(3)} = \frac{e}{3} \left[ 2 \left( \mathbf{K}_1^{(3)} \right) + \left| \mathbf{K}_1^{(3)} \right| + \left| \mathbf{K}_2^{(3)} \right| + \mathbf{P}^{(4)} \right] \quad \text{mod } e\mathbf{R}, \tag{A27}
\]

while for \( C_n \) with \( n = 4, 6 \), we can use the simplified expressions from Ref. [28]:

\[
\mathbf{P}^{(4)} = \frac{e}{2} \left( \mathbf{X}_1^{(2)} \right) (\mathbf{a}_1 + \mathbf{a}_2) \quad \text{mod } e\mathbf{R}, \tag{A28}
\]

\[
\mathbf{P}^{(6)} = 0 \quad \text{mod } e\mathbf{R}. \tag{A29}
\]

Here, \( \mathbf{a}_1 \) and \( \mathbf{a}_2 \) are lattice basis vectors and \( \mathbf{R} = m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2 \) with \( m_1, m_2 \in \mathbb{Z} \) is a general Bravais lattice vector.

We now briefly apply the symmetry-indicator formulas in Appendix A4 [Eq. (A29)] to show that the polarization jump \( \Delta \mathbf{P}^{(n)} \) associated with the TPPs in \( C_n \)-symmetric systems is always vanishing. First, for a TPP along the \( \Gamma \) line of a \( C_3 \)-symmetric system [cf. Eq. (A18)], we obtain from Appendix A4 the jump of the bulk polarization

\[
\Delta \mathbf{P}^{(3)} = -e (\Delta \# \Gamma_1^{(3)} + \Delta \# \Gamma_2^{(3)}) (\mathbf{a}_1 + \mathbf{a}_2) \quad \text{mod } e\mathbf{R}, \tag{A30}
\]

Similarly, for a TPP along the \( K \) line [cf. Eq. (A19)]

\[
\Delta \mathbf{P}^{(3)} = \frac{e}{3} (2 \Delta \# \mathbf{k}_1^{(3)} + \Delta \# \mathbf{k}_2^{(3)}) (\mathbf{a}_1 + \mathbf{a}_2) \quad \text{mod } e\mathbf{R}, \tag{A31}
\]

where we have read from Table IV that \( \Delta \# \mathbf{k}_1^{(3)} = 2 \) and \( \Delta \# \mathbf{k}_2^{(3)} = -1 \) for a TPP formed by ICRs (\( \mathbb{E}^\prime ; \mathbf{A}_1, \mathbf{A}_2 \)).

Furthermore, note that per Appendix A4 the polarization always vanishes in \( C_n \)-symmetric systems. Therefore, \( \Delta \mathbf{P}^{(n)} = 0 \) mod \( e\mathbf{R} \) for TPPs along both the \( \Gamma \) line [cf. Eq. (A20)] and the \( K \) line [cf. Eq. (A25)] of \( C_n \)-symmetric systems. Next, for TPPs along the \( \Gamma \) line of \( C_3 \)-symmetric systems [cf. Eq. (A23)] we find from Eq. (A28) that the change in bulk polarization is

\[
\Delta \mathbf{P}^{(4)} = -\frac{e}{2} \Delta \# \Gamma_1^{(2)} (\mathbf{a}_1 + \mathbf{a}_2) \quad \text{mod } e\mathbf{R}
\]

\[
= 0 \quad \text{mod } e\mathbf{R}, \tag{A32}
\]

where we have read from Table VI that \( \Delta \# \Gamma_1^{(2)} \) is even for all possible TPPs. Finally, note that TPPs along the \( M \) line [cf. Eq. (A24)] do not have an effect on the symmetry indicator \( |X_1^{(2)}| \) in Eq. (A28), therefore, again \( \Delta \mathbf{P}^{(4)} = 0 \) mod \( e\mathbf{R} \). We conclude that all TPPs listed in Table II are associated with no jump in surface charge, thus making the hinge-charge jump observable for an appropriate choice of the boundary termination.

**APPENDIX B: EULER MONOPOLE CHARGE IN THE PRESENCE OF ROTATIONAL SYMMETRY**

In this Appendix we derive the statements made in Sec. IV B and apply them to triple-point pairs (TPPs) to find the combinations of irreducible corepresentations (ICRs) that necessarily lead to a gapless bulk on at least one side of the TPP. Such TPPs cannot be associated with a higher-order signature on the wire hinges; for brevity, we call them inadmissible TPP configurations. For the remaining cases, we determine the value of the Euler monopole charge given in Table II. The analysis assumes the presence of space-time inversion (\( \mathbb{PT} \)) symmetry unless explicitly stated otherwise (a particular case of the latter is the entire Appendix B 5).

The presented arguments are based on analyzing the spectrum of Wilson-loop operators on certain appropriately chosen paths. The Wilson-loop operators are defined in terms of projectors onto occupied eigenstates \( |u_i(k)\rangle \) of the Bloch Hamiltonian \( \mathcal{H}(k) \). We organize the occupied eigenstates into an \( N \times N_{\text{occ}} \) matrix

\[
\mathbf{u}(k) = (|u_1(k)\rangle \ |u_2(k)\rangle \ldots |u_{N_{\text{occ}}}(k)\rangle), \tag{B1}
\]

where \( N \) is the total number of bands and \( N_{\text{occ}} \) is the number of occupied bands. In the presence of \( \mathbb{PT} \) symmetry satisfying \( \mathbb{PT} \mathbb{T} = -I \), we always adopt a basis of the Hilbert space in which \( \mathbb{PT} \) is represented by complex conjugation \( \mathcal{K} \). Then, the Bloch Hamiltonian is a real-symmetric matrix, and the eigenstates [as well as the matrix \( \mathbf{u}(k) \)] can be gauged to be real. To determine the advertised properties of TPPs, we need to study how the spectrum of the Wilson operator on certain appropriately chosen paths is constrained by \( \mathbb{PT} \), \( \mathbb{P} \), and \( C_n \) symmetries.

The discussion in this Appendix is structured as follows. In Appendix B 1 we study how \( C_n \) rotational symmetry constrains the Wilson-loop operator on an appropriately chosen path, composed of two \( C_n \)-related segments. Next, in Appendix B 2, we use the previous result to relate the Berry phase of the occupied bands on a particular choice of path to the \( C_n \) eigenvalues of the occupied bands at the high-symmetry line, and in Appendix B 3 we derive a symmetry-indicator formula for the Euler monopole charge. Then, in Appendix B 4, we apply the previous two results to TPPs, identifying which TPPs are inadmissible and giving the Euler monopole charge for each admissible TPP configuration. Finally, in Appendix B 5
we extend the discussion of inadmissible TPPs to systems without \(PT\) symmetry.

1. Symmetry constraint on Wilson-loop operator

We define the following family of closed contours

\[
\Gamma(\phi) = \gamma(\phi)^{-1} \circ \gamma(0)
\]

consisting of half circles given by \(\gamma(\phi) : \theta \in [0, \pi] \mapsto \gamma(\theta, \phi)\) with

\[
\gamma(\theta, \phi) = R \begin{pmatrix}
\sin(\theta) \cos(\phi) \\
\sin(\theta) \sin(\phi) \\
-\cos(\theta)
\end{pmatrix}
\]

(B3)

One example of such a contour is illustrated in Fig. 8 in green color. We abbreviate \(u(\theta, \phi) = u(\gamma(\theta, \phi))\), \(u_0 = u(0, \phi)\), and \(u_1 = u(\pi, \phi)\) for any \(\phi \in [0, 2\pi]\).

Given any closed path \(\Gamma(t)\) defined on \(t \in [0, 1]\), the Wilson-loop operator is defined by

\[
W(\Gamma)_{mn} = \lim_{\delta t \to 0} \left( u_m(\Gamma(1)) \prod_{t=0}^{1-\delta t} \mathbb{P}(\Gamma(t)) \right) u_n(\Gamma(0)).
\]

(B4)

where \(\delta t\) is the discretization of \(t\) in the product, the arrow over the product symbol indicates the ordering of the factors from small to large values of \(t\) (i.e., in this case factors with smaller \(t\) are to the right), and

\[
\mathbb{P}(k) = \sum_{j=1}^{N_{\text{occ}}} |u_j(k)\rangle \langle u_j(k)|
\]

(B5)

is the projector onto the occupied subspace. Observing that

\[
u(k)u(k)^\dagger = \sum_{j=1}^{N_{\text{occ}}} |u_j(k)\rangle \langle u_j(k)| = \mathbb{P}(k),
\]

(B6)

we can rewrite the expression for the Wilson-loop operator in matrix form (\(\mathbb{W}\) is an \(N_{\text{occ}} \times N_{\text{occ}}\) matrix)

\[
\mathbb{W}(\Gamma) = \lim_{\delta t \to 0} \mathbb{W}(\Gamma(1)) \prod_{t=0}^{1-\delta t} \mathbb{P}(\Gamma(t)) \mathbb{W}(\Gamma(0)).
\]

(B7)

The Wilson-loop operator for one of the closed contours \(\Gamma(\phi)\) defined above is then found to be

\[
\mathbb{W}(\phi) = \mathbb{W}(\Gamma(\phi)) = \lim_{\delta t \to 0} \mathbb{W}(\Gamma(1)) \prod_{t=0}^{1-\delta t} \mathbb{P}(\Gamma(t)) \mathbb{W}(\Gamma(0)).
\]

(B8)

Reordering the terms in the products, this becomes

\[
= \lim_{\delta t \to 0} \mathbb{P}(0) \mathbb{W}(\Gamma(1)) \prod_{t=0}^{1-\delta t} \mathbb{P}(\Gamma(t)) \mathbb{W}(\Gamma(0))
\]

(B9)

with

\[
V(\theta, \phi) = u(\theta + \delta \theta, \phi)^\dagger u(\theta, \phi)
\]

(B10)

If we choose the real gauge along \(\Gamma(\phi)\) by monodromy, \(V(\theta, \phi) \in SO(N_{\text{occ}})\).

The \(C_\pi\) rotational symmetry relates eigenstates at points in momentum space related by that symmetry:

\[
u(C_\pi k) = D(C_\pi)u(k)B(k),
\]

(B11)

where \(D(C_\pi)\) is the corepresentation matrix of \(C_\pi\) in the chosen basis, i.e., where \(D(PT) = 1\), and \(B(k) \in Q(N_{\text{occ}})\) is a sewing matrix [33]. Thus, for any \(\theta, \phi\),

\[
u \left( \theta, \phi + \frac{2\pi}{n} \right) = D(C_\pi)u(\theta, \phi)B(\theta, \phi).
\]

(B12)

Substituting this into the expression for the Wilson-loop operator, we find

\[
\mathbb{W}(\phi + \frac{2\pi}{n}) = \lim_{\delta t \to 0} \mathbb{W}(\Gamma(1)) \prod_{t=0}^{1-\delta t} \mathbb{P}(\Gamma(t)) \mathbb{W}(\Gamma(0))
\]

(B13)

where the sewing matrices canceled out. Reordering the terms again,

\[
\mathbb{W}(\phi + \frac{2\pi}{n}) = \lim_{\delta t \to 0} \mathbb{W}(\Gamma(1)) \prod_{t=0}^{1-\delta t} \mathbb{P}(\Gamma(t)) \mathbb{W}(\Gamma(0))
\]

(B14)

Note that

\[
u^\dagger(0)D(C_\pi)u_0 = D_0(C_\pi),
\]

(B15)

\[
u^\dagger(1)D(C_\pi)u_1 = D_1(C_\pi)
\]

(B16)

gives the corepresentation matrices \(D_{0,1}(C_\pi)\) of only the occupied bands at \(\Gamma(0)\) and \(\Gamma(1/2)\) (i.e., at the south and north pole, respectively. Thus,

\[
\mathbb{W}(\phi + \frac{2\pi}{n}) = \lim_{\delta t \to 0} D_0(C_\pi) \prod_{\theta} V(\theta, \phi)^\dagger D_1(C_\pi) \prod_{\theta} V(\theta, 0) u_0.
\]

(B17)

Defining

\[
P(\phi) = \prod_{\theta} V(\theta, \phi) \in SO(N_{\text{occ}}),
\]

we arrive at Eq. (9) of Sec. IV B:

\[
\mathbb{W}(\phi + \frac{2\pi}{n}) = D_0(C_\pi)P(\phi)^\dagger D_1(C_\pi)P(\phi)\mathbb{W}(\phi).
\]

(B18)
2. Berry phase on a symmetric path

The constraint on the Wilson-loop operator derived above has implications for the Berry phase of the occupied bands computed on the contours $\Gamma(\phi)$. The Berry phase is given by $\phi = \arg \det W$, such that

$$\phi \left( \frac{2\pi}{n} \right) = \arg \det \left[ D_0(C_n)P(\phi)^{\dagger}D_1(C_n)^{\dagger}P(\phi)W(\phi) \right].$$

Using that inside the determinant all matrices commute,

$$\phi \left( \frac{2\pi}{n} \right) = \arg \det W(\phi) + \arg \det \left[ D_0(C_n)D_1(C_n)^{\dagger} \right]$$

which is exactly Eq. (10). The difference in Berry phase on the two contours is found to be

$$\Delta \phi = \arg \det \left[ D_0(C_n)D_1(C_n)^{\dagger} \right].$$

Recall that in the presence of $PT$ symmetry, the Berry phase on any closed loop is (as well as their differences) quantized to $0$ vs $\pi$, and that the Berry curvature vanishes identically away from the nodal lines [68]. It therefore follows that the trivial value $\Delta \phi = 0$ indicates that there is an even number of nodal lines enclosed by the contour $\gamma(\phi + 2\pi/n)\circ \gamma(\phi)$, while a nontrivial value $\Delta \phi = \pi$ indicates an odd number. This implies that each $\frac{2\pi}{n}$ sector of the spherical surface is penetrated by an even (odd) number of nodal lines in the principal gap and thus, if $\Delta \phi = \pi$, that the surface must contain gapless points.

3. Symmetry indicators for Euler monopole charge

We now specialize to the case where $N_{\text{occ}} = 2$ and assume that $D_{0,1}(C_n) \in SO(2)$. Since the $n$th power of $D_{0,1}(C_n)$ gives the identity, it follows that for $j \in \{0, 1\}$,

$$D_j(C_n) = e^{-\frac{2\pi i j}{n}}$$

and Pauli matrices $s_i$ acting on the space of the two valence bands. Because $SO(2)$ is an Abelian group, we find that

$$W(\phi + \frac{2\pi}{n}) = D_0(C_n)D_1(C_n)^{\dagger} \lim_{\delta \theta \to 0} \left[ \prod_{\theta} V(\theta, \phi)^{\dagger} \right] \prod_{\theta} V(\theta, 0) u_0$$

$$= D_0(C_n)D_1(C_n)^{\dagger} W(\phi).$$

From the family of Wilson-loop operators $W(\phi)$ for $\phi \in [0, 2\pi)$, the Euler class can be obtained [73]. Since $W(\phi) \in SO(2)$, there is a $\zeta(\phi) \in [0, 2\pi)$ such that

$$W(\phi) = e^{i\zeta(\phi) s_y}.$$ 

given by the Pfaffian of the logarithm

$$\zeta(\phi) = \text{Pf} \left[ \log W(\phi) \right] \mod 2\pi.$$ 

The phase $\zeta(\phi)$ changes continuously in $\phi$ as long as the two-band subspace is separated from the other bands by energy gaps, and its winding number determines the Euler class as

$$\chi = \frac{1}{2\pi} \int_0^{2\pi} \frac{d\zeta(\phi)}{d\phi} = \frac{1}{2\pi} [\zeta(2\pi) - \zeta(0)].$$

We remark that the above expression should be read with caution. Namely, a gauge transformation $u_0 \mapsto u_0 U$ with $U \in O(2)$ at the base point of the closed path $\Gamma$ transforms the Wilson-loop operator as follows:

$$W(\phi) \mapsto U^\dagger W(\phi) U,$$

such that $\zeta(\phi) \mapsto \zeta'(\phi)$ with

$$\zeta'(\phi) = \text{Pf} \left[ \log U^\dagger W(\phi) U \right] \mod 2\pi$$

$$= \text{Pf} \left[ U^\dagger \log W(\phi) U \right] \mod 2\pi.$$ 

Using that $\text{Pf}(BAB^\dagger) = \text{det}(B)\text{Pf}(A)$, we obtain

$$= \text{det}(U) \zeta(\phi) \mod 2\pi.$$ 

Since $\text{det}(U) = \pm 1$, the sign of $\zeta(\phi)$ and therefore $\chi$ is gauge dependent [73]. Therefore, the well-defined topological invariant that we can extract is the absolute value $|\chi|$ of the Euler monopole charge.

Equation (B22) implies that

$$\zeta(\phi + \frac{2\pi}{n}) = \text{Pf} \left[ \log e^{\frac{i\pi}{n}(r_1 - r_0)s_y + i\zeta(\phi)s_y} \right]$$

$$= \frac{2\pi}{n} (r_1 - r_0) + \zeta(\phi) \mod 2\pi$$

and applying that identity $n$ times gives

$$\zeta(\phi + 2\pi) = 2\pi (r_1 - r_0) + \zeta(\phi) \mod 2\pi.$$ 

Therefore, the Euler class is

$$\chi = r_1 - r_0 \mod n.$$ 

Recall that the parity of $\chi$ is the second Stiefel-Whitney class $w_2 = \chi \mod 2$. 

Observe that, for odd $n$, Eq. (B30) leaves the parity of $\chi$ undetermined. It follows that for $C_3, w_2$ is not constrained by symmetry, which is consistent with what we demonstrated in Sec. V D.

4. Application to triple-point pairs

We apply the above results to TPPs formed by a 2D ICR $\rho^{2D}$ and two 1D ICRs $\rho^{1D}_a, \rho^{1D}_b$. In that case the representation matrices of $C_n$ in the orange and blue $k_z$ ranges appearing in Eqs. (B19) and (B30) are

$$D_0(C_n) = \rho^{2D}(C_n),$$

$$D_1(C_n) = \rho^{1D}_a(C_n) \oplus \rho^{1D}_b(C_n).$$

respectively. For the relevant point groups stabilizing TPPs in the presence of $PT$ symmetry, Table IX lists the representation matrices for all 1D and 2D ICRs.

In Appendix B 2 we have derived a necessary condition for the enclosing spherical surface (on which the Wilson-loop operators are computed) to be gapped. Substituting Eq. (B32) into Eq. (B19), we find that the condition

$$\arg \det \left[ \rho^{2D}(C_n)\rho^{1D}_a(C_n)^\dagger \oplus \rho^{1D}_b(C_n)^\dagger \right] = 0$$

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TABLE IX. Irreducible corepresentations (ICRs) of the C_n rotational symmetry in the point groups C_{n\nu}, with space-time inversion symmetry \mathcal{PT} for n \in \{3, 4, 6\}. The notation for the ICRs follows Ref. [65], where we drop the subscripts if they do not affect the result. Note that for the 2D ICRs of the point group C_{4(v)} we define \hat{E_2} \hat{E_1} \hat{E_1} \equiv E_1 and \hat{E_1} \hat{E_1} \hat{E_1} \equiv E_2. The 2D ICRs are all SO(2) matrices and are therefore given in the form \( e^{\pi i \phi} \) for \( r \in \mathbb{Z} \) and the Pauli matrix \( \gamma_y \).

| ICR \( \rho(C_n) \) | \( E_1 \) | \( E_2 \) |
|-----------------|--------|--------|
| \( (A, A) \)    | 1 \(-\pi/2\) | \( \pi/2\) |
| \( (B, B) \)    | 0 \(\pi/2\) | 0 \(\pi/2\) |

According to Table IX, all 2D ICRs have determinant 1, such that Eq. (B34) is violated by all combinations of ICRs that involve two 1D ICRs with different rotation eigenvalue. For \( C_4 \) symmetries this excludes \( (E; A, B) \) and for \( C_6 \) \((E; A, B)\) with \( i = 1, 2 \). (Note that we have dropped subscripts at A and B where they do not make a difference; this convention is also adopted in Tables II, IX, and X.)

Finally, we apply Eq. (B30) to all admissible combinations of ICRs from Table IX, i.e., where the 1D ICRs have equal rotation eigenvalues. In all those cases both \( \rho^{2D}(C_n) \) and \( \rho^D_a(C_n) \oplus \rho^D_b(C_n) \) are indeed SO(2) matrices. The results are shown in Table X. Note that (i) only the absolute value of the Euler class is well defined since the sign is gauge dependent, and (ii) the symmetry-indicator formula determines the Euler monopole charge modulo \( n \), where \( n \) is the order of the rotational symmetry. Due to these two ambiguities, \( \{0, 1, \ldots, [\frac{n}{2}]\} \) is the largest set of unique values of the Euler monopole charge that can be distinguished based on the ICRs of the two valence bands. More precisely, all values of \( \chi \) such that \( \chi = mn \pm p \) (with \( n \) the order of the rotational symmetry, \( p \) an element of the just specified set, and \( m \in \mathbb{Z} \)) are not distinguishable from \( \chi = p \). With the convention that \( a \mod n \in \{-[n/2], \ldots, [n/2]\} \), we write \( |\chi \mod n| \) to indicate the representative of the corresponding equivalence class of all such indistinguishable values of \( \chi \).

In particular, for \( n = 6 \), values \( |\chi| = 4 \) and \( |\chi| = 5 \) are indistinguishable from \( |\chi| = 2 \) and \( |\chi| = 1 \), respectively; while for \( n = 4 \), the value \( |\chi| = 3 \) is indistinguishable from \( |\chi| = 1 \). For these two cases the parity of \( \chi \) is well defined, such that the 2SW monopole charge, given by \( w_2 = \chi \mod 2 \in \mathbb{Z}/2\) \( \equiv 1 \), is uniquely determined. In contrast, for \( n = 3 \), the symmetry-indicator formula for \( \chi \) can only distinguish values \( |\chi| = 0 \) and \( |\chi| = 1 \), with \( |\chi| = 2 \) being indistinguishable from \( |\chi| = 1 \). This implies that the parity is not fixed by the symmetry indicators and therefore the 2SW monopole charge in \( C_3 \)-symmetric models is not determined from the symmetry eigenvalues.

| \( \chi \mod n \) | \( w_2 \) |
|--------------|--------|
| 1        | 1 \(\pi\) |
| 0 \(\pi\) | 0 \(\pi\) |

5. Gaplessness in absence of \( \mathcal{PT} \) symmetry

Here, we discuss the implications of Eq. (B19) (the derivation of which only assumes the \( C_n \) rotational symmetry) in the absence of \( \mathcal{PT} \) symmetry. By adjusting a few steps leading to Eq. (B20), one should recognize that the Berry phase on any closed loop of the form \( \Lambda(n, \phi) = \gamma(\phi + 2\pi/n)^{-1} \circ \gamma(\phi) \) (and assuming the trajectory does not encounter nodes in the principal gap) is given by

\[
\varphi_n = \arg \det[D_{0}(C_n)D_{1}(C_n)^{-1}],
\]

independent of \( \phi \). In the presence of \( \mathcal{PT} \), we have argued that the Berry phase on any closed path [including the phase \( \varphi_n \) on \( \Lambda(n, \phi) \)] is quantized to 0 vs \( \pi \), and that \( \varphi_n = \pi \) implies an odd number of nodal lines to pass through the loop. If \( \mathcal{PT} \) is absent but vertical mirror symmetries \( (m_x) \) are present, then an analogous quantization of Berry phase can be established for loops that are symmetric under mirror reflection [115–117], and nodal lines can only be stabilized inside mirror planes. In this case, a \( \pi \) Berry phase implies that the mirror-symmetric loop encloses an odd number of nodal lines inside the mirror-invariant plane. (The cases with neither \( \mathcal{PT} \) nor \( m_x \) are dealt with trivially towards the end of this section.)

In the relevant magnetic point groups with rotational symmetry \( C_n \), with vertical mirror symmetry, but without \( \mathcal{PT} \) symmetry (cf. Table I), we can therefore choose \( \phi \) such that

| \( \chi \mod n \) | \( w_2 \) |
|--------------|--------|
| 1        | 1 \(\pi\) |
| 0 \(\pi\) | 0 \(\pi\) |
By combining the previous two equations, we obtain

$$\varphi_n = (M_1 + M_2 \mod 2) \pi, \quad (B38)$$

meaning that $\varphi_n \in [0, \pi]$ determines the parity of the number of nodal lines in mirror planes $m_1$ and $m_2$ together, i.e., exactly the ones passing through a $\frac{2\pi}{m}$ sector of the enclosing sphere, just as in the presence of $\mathcal{PT}$ symmetry.

Let us finally remark that for TPs stabilized by $C_n\mathcal{PT}$ with $n = 4, 6$, we only need to consider the case with mirror symmetry because if no mirror symmetry is present, then nodal lines cannot be stabilized away from the rotation axis (see also the discussion in Sec. IV D). Therefore, there are no stable band nodes bound to the enclosing sphere. But, the case of $C_n\mathcal{PT}$ and mirror symmetry reduces to the case $C_n'$ with $n'/2 \in \{2, 3\}$ and mirror symmetry that we have discussed in the previous two paragraphs.

In conclusion, we have shown that even in the absence of $\mathcal{PT}$ symmetry,

$$\det \rho^{2D}(C_n) \neq \rho_{a,1D}(C_n)\rho_{b,1D}(C_n) \quad (B39)$$

implies that the bulk in the orange or blue $k_z$ ranges is necessarily gapless. It remains to check this condition for all possible combinations of ICRs. To that end, recall from Sec. IV D that in the presence of vertical mirror symmetry, addition of $\mathcal{PT}$ does not change the ICRs and Table IX still applies, giving the same result as in the presence of $\mathcal{PT}$. The only remaining cases are the magnetic point groups $42m$ and $6\bar{2}m2$. For the former we find $\det \rho^{2D}(C_4) = 1$, $\rho_{a,1D}(C_4) = 1$ and for the latter $\det \rho^{2D}(C_6) = 1$, $\rho_{a,1D}(C_6) = 1$, such that in both cases none of the combinations of ICRs are necessarily gapless.

APPENDIX C: TIGHT-BINDING MODELS

1. Construction of minimal tight-binding models

To construct the three tight-binding models discussed in Sec. V, we proceed as follows. We first choose a point group ($D_{4h}$ and $D_{6h}$ for our models) containing the little cogroup $G_k$ which we want to protect the triple points (TPs) as a subgroup. The choice of orbitals determines the irreducible representations of the point group. Using the 3D GENPOS application on the Bilbao crystallographic server (BCS), we determine a set of possible generators of that point group, and then find their matrix representations using the REPRESENTATIONS PG application [106]. To find the ICRs corresponding to the irreducible representations of the chosen orbitals after inclusion of $\mathcal{PT}$ symmetry with $(\mathcal{PT})^{-1} = +1$, we follow Ref. [65]. Given the set of generators, their ICRs and a generating set of hopping vectors, we use the Python package QSYM [118] to construct a family of symmetry-allowed Bloch Hamiltonians.

Finally, we tune the parameters in that family of Hamiltonians such that we obtain a four-band triple-point pair (TPP), accompanied by the minimal number of additional nodal lines (NLs). This is achieved by first introducing a double-band inversion at $\Gamma$ by setting selected intraorbital hopping parameters to be nonvanishing, and then by adding interorbital terms until we gap out all band nodes that are not required by the symmetry or topology. Note that the type of the TPs can be predicted using our previously developed classification [60].
Using topological quantum chemistry (TQC) and the BANDREP application on BCS [38,106,119], we deduce the ICRs at the high-symmetry points, and using the COMPATIBILITY relations [106] infer the ones along the relevant rotation axis.

2. Details of the discussed tight-binding models

Here, we provide details of the models studied in Sec. V. For each model we present the Hamiltonian, the basis in which the Hamiltonian is expressed, the numerical values of parameters considered in the main text, and the matrix representations that we used to construct the models (cf. Appendix C1).

a. $C_{6}$-symmetric model with two type-A triple points

The model discussed in Sec. VB has SG P6/mmm (No. 191) and is defined on a hexagonal lattice with lattice constants $a = c = 1$. As described in the main text, we place $(d_{xy}, d_{x^{2}-y^{2}})$, and $f_{x(3z^{2}-r^{2})}$, $f_{y(3z^{2}-r^{2})}$ orbitals at Wyckoff position (WP) 1a (site-symmetry group $D_{6h}$). We adopt the basis $(d_{xy}, d_{x^{2}-y^{2}}, f_{x(3z^{2}-r^{2})}, f_{y(3z^{2}-r^{2})})$, such that $\mathcal{P} \mathcal{T}$ is represented simply by complex conjugation. According to TQC such a placement of orbitals results in the irreducible representations $(E_{2g}; B_{1u}, B_{2u})$ of $D_{6h}$ with unchanged ICRs after adding $\mathcal{P} \mathcal{T}$. In the above basis, the generators of $D_{6h}$ have matrix representations

$$C_{6c} = \text{diag}(R(-2\pi/3), -\mathbb{1}_{\tau}), \quad (C1a)$$
$$m_n = \sigma_i \otimes \tau_z, \quad (C1b)$$
$$\mathcal{P} = \sigma_z \otimes \mathbb{1}_{\tau}, \quad (C1c)$$
$$\mathcal{P} \mathcal{T} = \mathcal{K}, \quad (C1d)$$

where $m_n : y \rightarrow -y$ and $R(\theta)$ is the 2D rotation matrix

$$R(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}. \quad (C2)$$

The Pauli matrices $\sigma_i$ act on the $d$ vs $f$ (i.e., angular momentum) degree of freedom, while $\tau_z$ act on the two-level degrees of freedom with a fixed angular momentum.

Including only the nearest neighbor in plane as well as the nearest vertical hopping terms, the model’s Bloch Hamiltonian can be written as

$$\mathcal{H}^{(6)}_{AA}(k) = -\left[ t_1 + \sqrt{3} t_2 \left( \cos k_x + 2 \cos \frac{k_x}{2} \cos \frac{\sqrt{3} k_y}{2} \right) \right]$$
$$\frac{\sqrt{3}}{2} + \left( t_3 \cos k_z \right) \gamma_{13} - t_4 \left( \gamma_{14} - \gamma_{25} \right)$$
$$- t_5 \left( \cos k_x - \cos \frac{k_x}{2} \cos \frac{\sqrt{3} k_y}{2} \right) \left( \gamma_{14} + \gamma_{25} \right)$$
$$- \sqrt{3} \sin \frac{k_x}{2} \sin \frac{\sqrt{3} k_y}{2} \left( \gamma_{15} - \gamma_{24} \right)$$
$$- 2 t_6 \left[ \sin k_x \left( 2 \cos \frac{k_x}{2} + \cos \frac{\sqrt{3} k_y}{2} \right) \gamma_1 \right.$$
$$\left. - \sqrt{3} \cos k_x \sin \frac{\sqrt{3} k_y}{2} \gamma_2 \right], \quad (C3)$$

with the gamma matrices defined in Sec. II. We set the model parameters to $t_1 = 3$, $t_2 = -\frac{1}{2}$, $t_3 = -2$, $t_4 = \frac{5}{3}$, $t_5 = -\frac{1}{3}$, and $t_6 = -\frac{1}{3}$ to obtain a double-band inversion at $\Gamma$ and no other band inversions. The resulting band structure is shown in Fig. 14(a).

b. $C_{6}$-symmetric model with two type-B triple points

The second $C_{6}$-symmetric model, discussed in Sec. VC, has the same space group (SG) P6/mmm (No. 191) and is also defined on a hexagonal lattice with lattice constants $a = c = 1$. However, the $d$ orbitals are replaced by $p$ orbitals, such that we place $(p_x, p_y)$ and $f_{x(3z^{2}-r^{2})}$, $f_{y(3z^{2}-r^{2})}$ at WP 1a. We adopt the basis $(ip_x, ip_y, if_{x(3z^{2}-r^{2})}, if_{y(3z^{2}-r^{2})})$. According to TQC, this results in the irreducible representations $(E_{1u}; B_{1u}, B_{2u})$ of $D_{6h}$, again with unchanged ICRs after adding $\mathcal{P} \mathcal{T}$. In the above basis, the generators of $D_{6h}$ have matrix representations

$$C_{6c} = \text{diag}(R(2\pi/6), -\mathbb{1}_{\tau}), \quad (C4a)$$
$$m_n = \text{diag}(\tau_x, -\tau_z), \quad (C4b)$$
$$\mathcal{P} = -\mathbb{1}_{\sigma} \otimes \mathbb{1}_{\tau}, \quad (C4c)$$
$$\mathcal{P} \mathcal{T} = \mathcal{K}, \quad (C4d)$$

where Pauli matrices $\sigma_i$ act on the $p$ vs $f$ (i.e., angular momentum) degree of freedom, while $\tau_z$ act on the two-level degrees of freedom with a fixed angular momentum.

The model’s Bloch Hamiltonian with only the nearest neighbor in plane and the nearest vertical hopping terms is

$$\mathcal{H}^{(6)}_{BB}(k) = -\left[ t_1 + \left( \cos k_x + 2 \cos \frac{k_x}{2} \cos \frac{\sqrt{3} k_y}{2} \right) \right]$$
$$\frac{\sqrt{3}}{2} + t_3 \cos k_z \gamma_{13} - t_4 (\gamma_{14} - \gamma_{25})$$
$$- t_5 \left( \cos k_x - \cos \frac{k_x}{2} \cos \frac{\sqrt{3} k_y}{2} \right) (\gamma_{14} + \gamma_{25})$$
$$- \sqrt{3} \sin \frac{k_x}{2} \sin \frac{\sqrt{3} k_y}{2} \left( \gamma_{15} - \gamma_{24} \right)$$
$$- 2 t_6 \left[ \left( \cos k_x - \cos \frac{k_x}{2} \cos \frac{\sqrt{3} k_y}{2} \right) \gamma_1 \right.$$
$$\left. - \sqrt{3} \sin \frac{k_x}{2} \sin \frac{\sqrt{3} k_y}{2} \gamma_2 \right], \quad (C5)$$

with the gamma matrices defined in Sec. II. We set the model parameters to $t_1 = 4$, $t_2 = -\frac{2}{3}$, $t_3 = -3$, $t_4 = -\frac{1}{3}$, $t_5 = -\frac{1}{3}$, and $t_6 = \frac{5}{3}$, which results in the band structure plotted in Fig. 15(a).

C. $C_{3}$-symmetric models

The $C_{3}$-symmetric models of Sec. WD are obtained by starting from either Eq. (C3) or Eq. (C5) and adding the
following perturbations to the Hamiltonian:

$$\Delta H^{(3)}_{\text{AA}}(k) = \delta_{C_3} \left( \begin{array}{cc} 1 & 0 \\ 0 & 0 \end{array} \right) \otimes \left[ -173 \sin k_x \\ 2 \sin \frac{k_y}{2} (58 \cos k_x + 115 \cos \sqrt{3} k_x) \right],$$

and

$$\Delta H^{(3)}_{\text{BB}}(k) = U_{\text{BB}} \Delta H^{(3)}_{\text{AA}}(k) U_{\text{BB}}^\dagger,$$

respectively, resulting in the Hamiltonians $H^{(3)}_{\text{AA}}(k)$ and $H^{(3)}_{\text{BB}}(k)$ whose NL structure is shown in Figs. 16(a) and 16(d), respectively. Note that, in contrast to the $C_6$-symmetric models, the subscript of the Hamiltonian does not denote the types of TPs because a $C_3$-symmetric little cogroup only allows for type-B TPs [60]. Instead, the subscript indicates from which $C_6$-symmetric model the corresponding $C_3$-symmetric model is derived.

APPENDIX D: COMPUTATION OF THE CORNER CHARGES

In this Appendix we provide technical details on some of the methods used in the extraction of the corner charges from the charge distribution obtained from exact diagonalization of the tight-binding models. First, note that if the electronic or ionic charge distribution leads to finite charge on different Wyckoff positions in the unit cell, we are left with an ionic crystal [88]. Therefore, a coarse graining or smoothing via a moving average is necessary to properly define edge and surface charge. In Appendix D1 we present a discrete method that performs this task. We used this method for the analysis of the models discussed in Secs. V and VIA. However, while this coarse graining easily removes strong oscillations of the charge distribution on sub-unit-cell length scales, oscillations due to trivial edge-localized states can remain [29] and obscure the corner charge. Therefore, in Appendix D2 we discuss a method that we developed to remove the signal due to such edge states. The method applies to the case when the total edge charge per unit cell (of the ribbon, i.e., the collection of sites periodically repeated in the ribbon geometry) is vanishing, but the presence of edge-localized states induces a nontrivial profile of the charge density as a function of the distance to the boundary, as has been observed for $\text{Sc}_3\text{AlC}$ in Sec. VIA.

1. Coarse graining of charge distribution

To coarse grain the electric charge distribution defined on the original lattice, we first need to choose the target lattice. The choice of target lattice defines the coarse-graining length scale. To coarse grain over a single unit cell with multiple sites, it is convenient to consider a single Wyckoff position of maximal symmetry to define the target lattice. Some examples are shown in Fig. 23. Note that it is also possible to coarse grain over larger lengths scales, i.e., multiple unit cells. Such a situation is depicted in Fig. 23(c) where coarse graining is performed over seven original hexagonal unit cells. However, note that due to overlapping of the coarse-graining cells, the Wigner-Seitz tessellation formed around the coarse-graining centers (not illustrated) coincides with the original honeycomb lattice.

The coarse graining is performed by redistributing the charge from the original to the target lattice. If a site on the original lattice belongs to $m$ coarse-graining cells, then a fraction $\frac{1}{m}$ of the total charge on the original site is distributed to each of the corresponding target sites. Consequently, charge on corner sites is generally transferred to a single target site. In Fig. 23(a), where we illustrate the coarse graining as applied to $\text{Sc}_3\text{AlC}$, redistribution weights of magnitude $1, \frac{1}{2},$ and $\frac{1}{3}$ are illustrated with solid, dashed, and dotted arrows, respectively.

We have applied the coarse-graining method to achieve a charge redistribution in all the discussed models. In particular, Fig. 13 shows a comparison of the charge distribution before [Figs. 13(a) and 13(b)] and after [Figs. 13(c) and 13(d)] coarse graining for the $C_3$-symmetric model of Sec. II. The definitions of the original and target lattice as well as the coarse-graining unit cell are shown in Fig. 23(b). Figures 23(a) and 23(c) give the same information for the model

![Fig. 23. Discrete coarse-graining method. (a) The charge on the original lattice (defined by the unit cells shaded in blue and sublattice sites shown as green disks) is redistributed to the target lattice (defined by the red diamond sites). Here the lattice corresponding to the projection of $\text{Sc}_3\text{AlC}$ (see Sec. VIA) is shown. Each site in the target lattice is assigned a coarse-graining cell (unit cell of that lattice; shaded in orange). The charge on each green site is then redistributed (black arrows) with equal weights (weight 1 shown by solid, $\frac{1}{2}$ by dashed, and $\frac{1}{3}$ by dotted lines) to all those red sites whose coarse-graining cell is adjacent to the green site. Only a few arrows are shown to maintain clarity of the illustration. (b), (c) Definitions of the original (green) and target (red) lattice and the coarse-graining cell (orange) for the $C_3$- and $C_6$-symmetric models discussed in Sec. V, respectively. Note that in (c) the coarse-graining cells overlap; as a consequence, the original and the target lattice coincide except for a missing layer on the boundary.](image-url)
FIG. 24. Procedure to remove the edge signal from the charge distribution of a \( C_4 \)-symmetric system. It is assumed that the total edge charge per unit cell (of the ribbon geometry) vanishes. The solid lines in both panels represent the boundary of the lattice. (a) Ribbon geometry extended in the horizontal direction with \( 2N - 1 = 7 \) unit cells in the vertical direction (corresponding to \( N = 4 \) inequivalent layers). Unit cells of the lattice are indicated by dots, colored according to their distance to the boundary. We denote by \( q_i \) the charge per unit cell on the \( i \)th layer (which is constant within the layer). (b) Flake geometry for the same system. Here, shells of unit-cell sites (dots) correspond to the layers from the ribbon geometry (indicated by the corresponding color). The charge on the whole flake is redistributed according to the arrows indicated in the bottom-left part of the system. The amount of charge that is transferred from a site that belongs to the \( j \)th shell to the next one is given by \( \sum_{i=1}^{N-1} q_i \), where \( q_i \) are the charges determined in the ribbon geometry [cf. (a)]. Note that the charge redistribution flows perpendicular to the boundary; therefore, no charge is transferred between the corners.

2. Removal of edge signal from charge distribution

Even after coarse graining (as described above), charge oscillations caused by trivial edge-localized states can remain. Note that in contrast to the oscillations on sub-unit-cell scale, these remaining oscillations are generally perpendicular to the edges, and vanish in the bulk. Since the total corner and edge charges are defined via integration over regions with boundaries perpendicular to the edges of the sample [29], the remaining oscillations do not prevent us from computing these total charges [see Fig. 18(c) for such a calculation on the original coarse-grained data]. However, such oscillations can visually obscure the localization properties of the charge. Here, we discuss a method to subtract such edge-localized oscillations for the cases where the total edge charge per unit cell (of the ribbon geometry) vanishes. The method applies to \( C_n \)-symmetric systems with \( n \geq 3 \), where the bulk as well as the finite-size sample satisfy the symmetry requirement. For concreteness we choose \( n = 4 \) for the following discussion. In particular, the described setup directly applies to the case of \( \text{Sc}_3\text{AlC} \) as presented in Sec. VI A.

Two separate calculations need to be performed: one on a ribbon with \( 2N - 1 \) layers (of unit cells) [cf. Fig. 24(a)] and one on a flake with \( N \) shells (of unit cells) [cf. Fig. 24(b)], such that there is a direct correspondence between the layers and the shells. Due to the rotational symmetry, the four sides of each shell are equivalent and only a single orientation of the ribbon needs to be computationally modeled. Note that compatible fillings (in particular, the same choice of chemical potential) need to be considered for the two systems. The charge distributions obtained for both geometries first need to be coarse grained to the level of unit cells (cf. Sec. VI A), such that the coarse-grained lattice has a single site per unit cell. The resulting lattices are depicted in Figs. 24(a) and 24(b).

From the calculation on the ribbon, the total charge \( q_{\mathrm{rip}} \) per unit cell in the \( i \)th layer can easily be extracted. On the flake, we then redistribute the charge as indicated in Fig. 24 with arrows: from a site in the \( j \)th shell (but not on one of the diagonals) the charge \( \sum_{i=1}^{j} q_i \) is transferred to the \( (j + 1) \)th shell. There is no charge transfer away from sites that lie on one of the diagonals. Therefore, this procedure seemingly leads to a charge accumulation on the diagonals and in the center. However, recall that, by assumption, the total edge charge

of Sc3AlC (cf. Sec. VI A) and the \( C_4 \)-symmetric models (cf. Secs. VB and VC), respectively.

TABLE XI. Compounds with space-time inversion symmetry that host type-A triple points (TPs) on the given high-symmetry line (HSL) and are therefore candidates for having a nontrivial Euler monopole charge. Some compounds host multiple TPs. For each material and TP the space group, the HSL on which the TP lies, the nodal-line (NL) segment carrying the Euler monopole charge, i.e., the segment enclosed by the ellipsoid, the relevant Berry phases, and the Euler monopole charge induced from Wilson-loop spectra are shown.

| Material | SG | HSL | NL segment | \( \phi_B \) | \( \chi \) |
|----------|----|-----|------------|------|-----|
| Na2LiN   | 129 | \( \Gamma - Z - \Gamma \) | [-0.29, 0.29] | (0, \( \pi \)) | 2 |
|          |     |     | [0.29, 0.71] | (\( \pi \), 0) | 2 |
| Li2NaN [91] | 191 | \( \Gamma - A - \Gamma \) | [-0.08, 0.08] | (0, 0) | 0 |
|          |     |     | [0.08, 0.92] | (0, \( \pi \)) | 2 |
| TiB2 [56] | 191 | \( \Gamma - A - \Gamma \) | [-0.26, 0.26] | (0, \( \pi \)) | 2 |
FIG. 26. Computation of Euler monopole charges of a pair of single triple points in Na$_2$LiN with the surface centered at $\Gamma$. (a) Shows the Brillouin zone, the high-symmetry points, and the planes in which the nodal lines are shown in (b). (b) Size of the four relevant gaps (orange, red, blue, and purple, according to increasing energy; at the triple point both the red and blue gaps are closed) in the two mirror planes shown in (a) encoded by the intensity of the color (and with a cutoff at a gap of 0.02 eV). The triple point (yellow) and the central nodal line are emphasized by appropriately colored overlays. (c) Wilson-loop spectrum computed for the relevant bands on the ellipsoid indicated in (b). We observe that the Wilson-loop spectrum winds twice, which implies $|\chi| = 2$.

vanishes, such that in the limit of large $N$, $\sum_{i=1}^{N} q_i = 0$. Consequently, the accumulated charge compensates oscillations on the diagonals and converges to zero at the center of the flake. Furthermore, note that the charge redistribution flows strictly perpendicular to the flake boundaries; therefore, no charge is transferred between the corners of the flake, keeping its value invariant (up to corrections that are exponentially small in the system size).

The effect of the method can be seen in Fig. 18, where the original (coarse-grained) distribution is shown in Figs. 18(d) and 18(e), and the charge distribution after removing the edge signal is displayed in Figs. 18(f) and 18(g). We remark that the data in Figs. 18(f) and 18(g) have undergone one additional coarse-graining step after the removal of the edge charge. Compared to Fig. 18(d), the localization of the corner charge in Fig. 18(f) is visually much more manifest.

APPENDIX E: GENERALIZED QUATERNION CHARGE IN DIFFERENT BRILLOUIN ZONES

In this Appendix we formalize the relationship between the orientation of nodal lines (NLs) and their copies in neighboring Brillouin zones (BZs). The orientation of a NL as used in Sec. III B can be formally defined using the non-Abelian invariant introduced by Ref. [66] (also called generalized quaternion charge therein). While the topological classification of band nodes is given by equivalence classes of the generalized quaternion group (each equivalence class contains either a single element or two elements that differ by a sign), the sign of the invariant becomes well defined if the contours have a common base point. In that case the sign of the generalized quaternion invariant computed on a contour enclosing a single NL defines [71] the orientation of that NL (cf. Fig. 25).

The prior works [66, 71] on the non-Abelian band topology have only considered closed contours which are fully contained within a single BZ. However, to understand the reversal of NL orientation between neighboring copies of BZ (cf. Fig. 6), one must explicitly consider paths that cross the BZ boundary. Such paths entail additional complications, as is well known from the case of the Zak-Berry phase [79, 120]; namely, in general $H(k)$ and $H(k + b)$, where $b$ is any reciprocal lattice vector, are not identical, but are related by a diagonal unitary rotation. In the Supplemental Material [72] we explain how to compute the non-Abelian invariant in that case and then prove a very general statement relating the values of the invariant computed on contours shifted by a reciprocal lattice vector but connected to a common base point (see, e.g., the light and dark green paths $\gamma$ and $\tilde{\gamma}$ in Fig. 25).

FIG. 27. Computation of Euler monopole charges of a pair of single triple points in Na$_2$LiN with the surface centered at $Z$. The organization of the panels is in one-to-one correspondence with Fig. 26 (the same cutoff of 0.02 eV is used). In (c) we observe that the Wilson-loop spectrum winds twice, which implies $|\chi| = 2$. 

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As a corollary of that general statement, we find that the following holds:

**Corollary 1.** Assume an $N$-band system with $PT$ symmetry squaring to $+1$ described in the orbital basis by a Hermitian Bloch Hamiltonian $H(k)$. Let $\gamma: t \in [0, 1] \mapsto \gamma(t)$ be a closed contour with no band degeneracies located inside the (first) BZ. The path starts at the base point $P = \gamma(0) = \gamma(1)$ and we decompose
\[
q(\gamma) = s \prod_{j \in J} g_j
\]
with $s \in \{\pm 1\}$, $g_j$ the generators defined in Refs. [60,66], and $J \subseteq \{1, 2, \ldots, N-1\}$ a subset of the energy gaps of the $N$-band Hamiltonian (factors with smaller subscript $j$ appearing to the right). Then, the generalized quaternion charge on the corresponding contour $\tilde{\gamma}$ with the same base point and enclosing the same band inversions but in the BZ shifted by the reciprocal lattice vector $b$ (cf. Fig. 25) is
\[
q(\tilde{\gamma}) = (-1)^m q(\gamma),
\]
where $m$ is the number of elements of the set
\[
\{ j \in J | \phi_j \neq \phi_{j+1} \}
\]
with $\phi_j \in [0, \pi)$ the Berry phase of the $j$th band in the direction $b$. [Note that in the conditioning in Eq. (E3) the label $j+1$ may not be in the set $J$.]

We briefly discuss the application of Corollary 1 to the situation discussed in Sec. III B and depicted in Fig. 6. We are interested in the change of the orientation of the blue nodal ring when comparing two copies displaced by the primitive reciprocal lattice vector in $k_z$ direction. Recall that the orientation of nodal lines (NLs) is defined via the generalized quaternion invariant of unique paths encircling those NLs with a fixed base point. This is exactly the situation of Corollary 1 with $q(\gamma) = s_g^2$ (in the figure the case $s=+1$ is illustrated). Then, the corollary implies that the orientation changes if and only if the Berry phases of bands 2 and 3 are different, i.e., if $\phi_2 + \phi_3 = \pi \mod 2\pi$, in agreement with the statements in the main text. We also remark that if $q(\gamma) = \pm 1$ (i.e., if the Berry phase of each band on $\gamma$ is trivial and no NLs are enclosed by $\gamma$), we have $J = \emptyset$ and Corollary 1 therefore immediately implies that $q(\gamma) = q(\tilde{\gamma})$.

**APPENDIX F: ADDITIONAL MATERIAL EXAMPLES WITH EULER MONOPOLE CHARGE**

From the list of triple-point (TP) materials in Ref. [59], we select additional candidates (aside from Li$_2$NaN) that potentially host TP-induced Euler monopole charges, namely, Na$_2$LiN, Li$_2$NaN, and TiB$_2$. Based on the first-principles calculations performed in Ref. [59] (and whose results are
which implies of the panels is in one-to-one correspondence with Fig. 26 (cutoff 0.05 eV). In (c) we observe that the Wilson-loop spectrum winds twice, which implies $|\chi| = 2$.

given in the corresponding supplemental data and code [121]), we construct maximally localized Wannier functions using WANNIER90 [97] with $s$ orbitals of alkali-metal elements, $d$ orbitals of transition metal elements, and $p$ orbitals of non-metal elements (for Li$_2$NaN no orbitals of Li are included). For the resulting Wannier tight-binding models we use the Python package Z2PACK [100,101] to compute the Wilson-loop spectra on ellipsoids enclosing the appropriate NL segments as well as the relevant Berry phases (cf. Fig. 6).

The results are summarized in Table XI and in Figs. 26–30 we show for each TP material and NL segment the resulting Wilson-loop spectrum from the value $\chi$ of the Euler monopole charge is deduced. By comparing the Berry phases and the values of the Euler monopole charge, we verify the condition for nontrivial Euler monopole charge discussed in Sec. III B. We provide access to the Wannier tight-binding models as well as the Wilson-loop spectra in the supplementary data and code [114].
