

Higher-order topological phases: A general principle of construction

Dumitru Călugăru,^{1,2} Vladimir Juričić,³ and Bitan Roy¹

¹Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Strasse 38, 01187 Dresden, Germany

²Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

³Nordita, KTH Royal Institute of Technology and Stockholm University, Roslagstullsbacken 23, 10691 Stockholm, Sweden



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We propose a general principle for constructing higher-order topological (HOT) phases. We argue that if a D -dimensional first-order or regular topological phase involves m Hermitian matrices that anticommute with additional $p - 1$ mutually anticommuting matrices, it is conceivable to realize an n th-order HOT phase, where $n = 1, \dots, p$, with appropriate combinations of discrete symmetry-breaking Wilsonian masses. An n th-order HOT phase accommodates zero modes on a surface with codimension n . We exemplify these scenarios for prototypical three-dimensional gapless systems, such as a nodal-loop semimetal possessing $SU(2)$ spin-rotational symmetry, and Dirac semimetals, transforming under (pseudo)spin- $\frac{1}{2}$ or 1 representations. The former system permits an unprecedented realization of a fourth-order phase, without any surface zero modes. Our construction can be generalized to HOT insulators and superconductors in any dimension and symmetry class.

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Topological phases of matter are characterized by the topological invariant of the corresponding bulk band structure, manifesting through metallic surface states. The bulk-boundary correspondence is operative for both gapped (insulators and superconductors) as well as gapless systems. Topological invariants protecting these boundary modes may arise solely from antiunitary (such as time-reversal, particle-hole) symmetries, as in quantum spin Hall insulators, or their combinations with unitary (such as crystalline) symmetries, as in topological crystalline insulators, or by no symmetry at all, as in quantum Hall or Chern insulators [1–11].

Recently, the notion of topological states of matter has been extended to include their higher-order cousins [12,13]. Prototypical examples include higher-order topological (HOT) insulators [12,14–34], superconductors [16,24,31,35–37], and semimetals [23]. A D -dimensional n th-order bulk topological phase hosts gapless states on a surface with codimension $d_c = n$, and bismuth (Bi) has emerged as a prominent candidate for a HOT insulator [26]. In this classification scheme, conventional topological phases are first order in nature. Recall that a three-dimensional “first-order” strong Z_2 topological insulator supports two-dimensional gapless surface states ($d_c = 1$), whereas its second-order and third-order realizations respectively accommodate one dimensional hinge modes with $d_c = 2$ (see Fig. 1) and pointlike corner states with $d_c = 3$. The present work promotes a general principle for constructing HOT phases, based on the dimensionality and symmetries of the system. For concreteness, we focus on prototypical gapless phases in three dimensions, such as Dirac and nodal-loop semimetals, and systematically construct their higher-order realizations. The central outcomes are summarized in Figs. 2–4.

To set the stage, we begin by recalling that the unstable fixed point separating two topologically distinct gapped phases (belonging to any Altland-Zirnbauer class in any dimension [38,39]) is described by massless Dirac fermions

[40,41]. The fundamentally important element in this construction is the topological Wilson mass, which introduces a nontrivial band gap for Dirac quasiparticles. Now, depending on the dimensionality and symmetry of the system, one can find several candidates for the topological mass, represented by mutually anticommuting Dirac matrices. For example, a four-component Dirac Hamiltonian in $D = 3$ (suitable to describe both topological insulators and superconductors) permits one time-reversal symmetry (\mathcal{T}) preserving ordinary Dirac mass and a \mathcal{T} -odd axion mass. Often the \mathcal{T} invariant Dirac mass constitutes a first-order topological insulator or superconductor, accommodating two-dimensional gapless surface states. The presence of the additional \mathcal{T} -odd Dirac mass then either (a) completely gaps the surface states, yielding an axionic insulator [42–44] or superconductor [45], when it is uniform (following the trivial representation) or (b) gives birth to one-dimensional hinge modes, when it also lacks certain discrete symmetry (such as C_4 , hence transforming under a nontrivial representation of lattice point group). The system then describes a second-order topological insulator or superconductor. Hence, the arena of the HOT phases (including insulators, superconductors and semimetals) can be ventured in terms of available “masses” for gapless Dirac fermions. Below, we formulate a general principle of constructing a hierarchy of HOT phases.

Let us assume that the minimal model describing a first-order topological phase involves m (often, but not necessarily, mutually anticommuting) Hermitian matrices. If there exist maximal $p - 1$ (≥ 0) mutually anticommuting matrices that also anticommute (hence represent mass orders) with the m matrices, then it is conceivable to realize up to an n th-order HOT phase, with appropriate combinations of n discrete symmetry-breaking Wilsonian masses, where $n = 1, \dots, p$. For the above example of a topological insulator or superconductor in $D = 3$ (described by four-component Dirac fermions), $m = 4$ and $p = 2$, and at most a second-order HOT

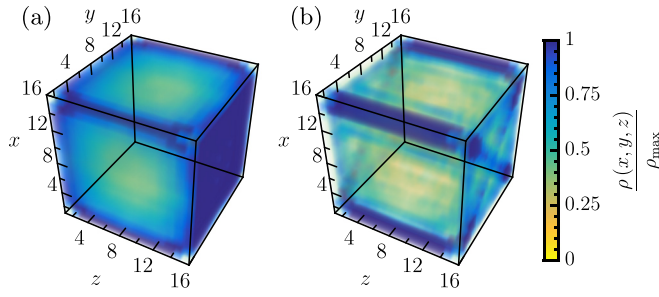


FIG. 1. Boundary modes of (a) first-order (occupying six surfaces) and (b) second-order (occupying four hinges) topological Kondo insulators, obtained from an appropriate tight-binding model for its prototypical representative SmB_6 [46].

phase can be realized in the presence of discrete symmetry-breaking axion mass. Within this framework we construct a second-order topological Kondo insulator (supporting four hinge modes) in the presence of a time-reversal symmetry-breaking quadrupolar Kondo singlet mass [see Fig. 1(b)] [46]. For rest of this Rapid Communication, we focus on topological semimetals and anchor this prediction for the following systems.

(1) Topological Dirac semimetals (TDSMs), transforming under either (pseudo)spin- $\frac{1}{2}$ or 1 representation, for which $m = 3$ and $p = 3$: We construct first-, second-, and third-order TDSMs, respectively supporting two-dimensional Fermi arcs, one-dimensional hinge, and zero-dimensional corner states (see Figs. 2 and 3). These conclusions remain operative for TDSMs, following any half-integer or integer (pseudo)spin representation [46].

(2) Nodal-loop semimetal (NLSM) with $\text{SU}(2)$ spin-rotational symmetry, for which $m = 2$ and $p = 4$: Consequently, we can find up to fourth-order NLSM (see Fig. 4). A fourth-order NLSM does not support any surface zero modes, since $d_c > D$ [46].

In the above examples of higher-order topological semimetals (HOSMs), the discrete symmetry-breaking Wilson masses, the key ingredient for the realization of any HOT phase, leave the topological band touching points unchanged [46].

We begin the journey through the territory of HOSMs with TDSMs, following a spin- j (half-integer or integer) representation. The Hamiltonian operator is given by

$$\hat{h}_j^{\text{Dirac}} = t \left[\tau_3 \otimes S_1^j N_1(\mathbf{k}) + \tau_0 \otimes \sum_{m=2}^3 S_m^j N_m(\mathbf{k}) \right], \quad (1)$$

where S_m^j are the standard $(2j+1)$ -dimensional spin- j matrices, t is the hopping amplitude, and

$$\begin{aligned} N_1(\mathbf{k}) &= \sin(k_x a), & N_2(\mathbf{k}) &= \sin(k_y a), \\ N_3^1(\mathbf{k}) &= \cos(k_z a) + [\cos(k_x a) + \cos(k_y a) - 2]. \end{aligned} \quad (2)$$

The Pauli matrices $\{\tau_\mu\}$ operate on the (pseudo)spin indices. For an arbitrary half-integer spin Dirac system, the energy spectra display multifringence with $(2j+1)$ effective Fermi velocities, and Kramers or (pseudo)spin degenerate, linearly dispersing valence and conduction bands touch each other

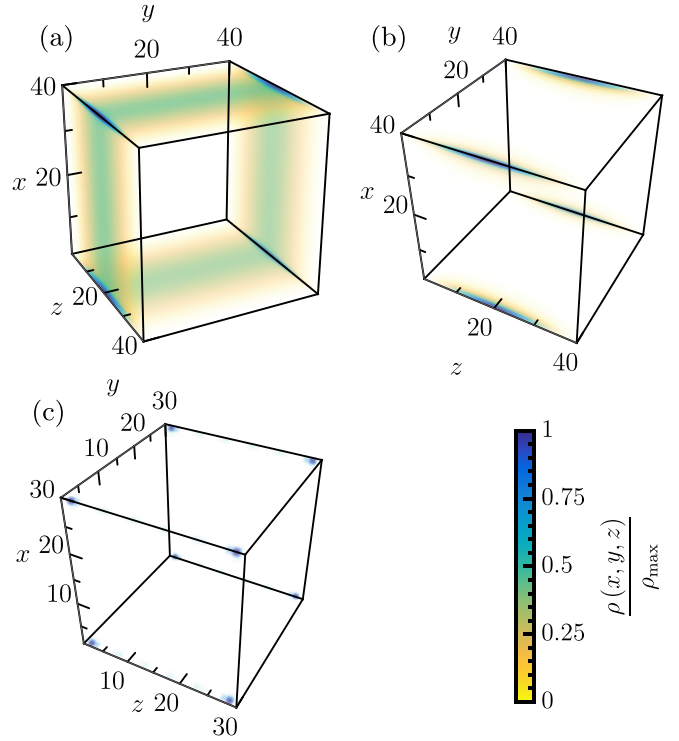


FIG. 2. (a) Two-dimensional Fermi arc surface states of a first-order, (b) four one-dimensional hinge states of a second-order, and (c) eight zero-dimensional corner states of a third-order spin- $\frac{1}{2}$ topological Dirac semimetal. We compute the square of the amplitude of the lowest-energy [$O(10^{-3}t)$ roughly] state $\rho(x, y, z)$ (normalized within the interval $[0, 1]$) on a cubic lattice with open boundaries in all three directions. For numerical diagonalization we set $t = 1$, $\Delta_1 = \Delta_2 = 0.3$ [46].

at $\mathbf{k} = (0, 0, \pm \frac{\pi}{2a})$, the Dirac points. Integer-spin Dirac systems additionally accommodate a pair of completely flat, but topologically trivial, bands precisely at zero energy. For concreteness, we here focus on TDSMs following $j = \frac{1}{2}$ and 1 representations.

TDSMs can be constructed by stacking two-dimensional quantum spin Hall insulators in the momentum space along, for example, the k_z direction. Each two-dimensional layer accommodates one-dimensional gapless edge modes in the xy plane. The resulting TDSMs then accommodate delocalized zero-energy surface states, but only on the xz and yz planes [see Figs. 2(a) (for spin- $\frac{1}{2}$) and 3(a) (for spin-1)], yielding topologically protected Fermi arcs (localized in the reciprocal space) [47, 48].

Higher-order TDSMs can be realized by introducing the following two discrete symmetry-breaking masses,

$$\hat{h}_{\text{XY-WDW}}^{\text{Dirac}, j} = \left[\sum_{j=1}^2 \Delta_j \tau_j N_j'(\mathbf{k}) \right] \otimes M_j, \quad (3)$$

where M_j is a $(2j+1)$ -dimensional *antidiagonal* identity matrix. In particular, we choose

$$\begin{aligned} N_1'(\mathbf{k}) &= \cos(k_x a) - \cos(k_y a) \sim k_x^2 - k_y^2 : B_{1g}, \\ N_2'(\mathbf{k}) &= \sin(k_x a) \sin(k_y a) \sin(k_z a) \sim k_x k_y k_z : B_{1u}, \end{aligned} \quad (4)$$

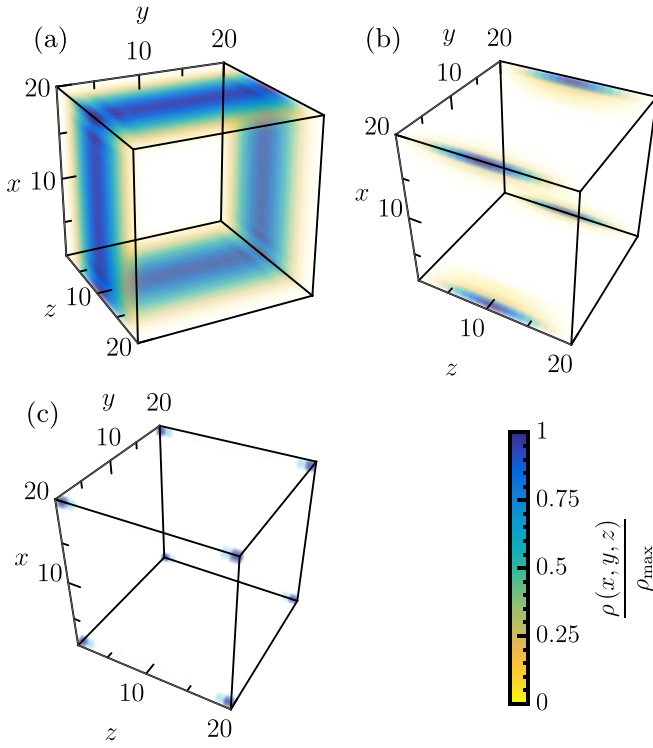


FIG. 3. Same as Fig. 2, but for spin-1 topological Dirac semimetals. For numerical diagonalization we set $\Delta_1 = 0.2$ for (b), and $\Delta_1 = 0.1$, $\Delta_2 = 0.2$ for (c). In (a) and (b) [(c)] we show the low-energy states maximally localized on the surface [at the corners] [46].

respectively transforming under the B_{1g} and B_{1u} representations of the tetragonal point group (D_{4h}). These two orders mix the in-plane components of (pseudo)spin, and we name them the XY Wilsonian density wave (XY-WDW). Note that $N'_1(\mathbf{k})$ and $N'_2(\mathbf{k})$ respectively represent quadrupolar and octupolar orders, but both of them vanish at $\mathbf{k} = (0, 0, \pm \frac{\pi}{2a})$. Hence, they do not affect the band-touching points, but for integer-spin systems, trivial flat bands acquire dispersion away from the Dirac points [46]. We first introduce the B_{1g} XY-WDW.

Notice that the B_{1g} XY-WDW order acts as a mass for the one-dimensional edge states associated with each copy of the two-dimensional spin Hall insulator, but changes sign under the C_4 rotation. The system can then be described as a collection of one-dimensional Dirac fermions (for each slice along the z direction) in the presence of a domain wall mass. The Jackiw-Rebbi index theorem [49] then guarantees the existence of precisely one zero-energy mode at four hinges between the xz and yz planes. A collection of such zero-energy modes constitutes four hinge states, as shown in Figs. 2(b) and 3(b), and a second-order TDSM is realized.

The B_{1u} XY-WDW acts as a mass for the one-dimensional hinge states of the second-order TDSM, but assumes the profile of a domain wall along the z direction. Therefore, a subsequent addition of the B_{1u} XY-WDW causes further dimensional reduction of the hinge modes, giving rise to eight corner states [see Figs. 2(c) and 3(c)] and a third-order TDSM is realized.

We now focus on a NLSM possessing an exact $SU(2)$ spin rotational symmetry. The Hamiltonian operator is given by

$$\hat{h}_0^{\text{NL}} = \sigma_0 \otimes \left[t \sum_{i=1}^2 N_i(\mathbf{k}) \tau_i \right]. \quad (5)$$

Two sets of Pauli matrices $\{\sigma_\mu\}$ and $\{\tau_\mu\}$ respectively operate on the spin and sublattice indices. The spinor basis is $\Psi_{\mathbf{k}}^\top = (\Psi_{\mathbf{k},\uparrow}, \Psi_{\mathbf{k},\downarrow})$, with $\Psi_{\mathbf{k},\sigma}^\top = (c_{\mathbf{k},\sigma}^A, c_{\mathbf{k},\sigma}^B)$ for two projections of electron spin $\sigma = \uparrow, \downarrow$. Here, $c_{\mathbf{k},\sigma}^X$ is the fermionic annihilation operator on sublattice $X = A, B$, with momentum \mathbf{k} and spin projection σ . We choose [50]

$$\begin{aligned} N_1^1(\mathbf{k}) &= \cos(k_x a) + \cos(k_y a) - b, \\ N_1^2(\mathbf{k}) &= \cos(k_z a) - 1, \quad N_2(\mathbf{k}) = \sin(k_z a), \end{aligned} \quad (6)$$

with $N_1(\mathbf{k}) = N_1^1(\mathbf{k}) + N_1^2(\mathbf{k})$ and $b < 2$. Here, $N_1^2(\mathbf{k})$ plays the role of a regular Wilson mass (preserving all symmetries) that removes the nodal loops at $k_z = \pm \frac{\pi}{a}$, leaving the one at $k_z = 0$ untouched. The inversion symmetry \mathcal{P} , under which $\mathbf{k} \rightarrow -\mathbf{k}$ and $\Psi_{\mathbf{k}} \rightarrow \tau_1 \Psi_{-\mathbf{k}}$ ensures the stability of the nodal loop in the $k_z = 0$ plane. The anticommutation relation $\{\tau_3, \hat{h}_0^{\text{NL}}\} = 0$ guarantees the spectral symmetry and spin-degenerate drumhead surface states are pinned at precisely zero energy on two opposite surfaces along the (001) direction [see Fig. 4(a1)]. The corresponding local density of states (LDOS) in the xy plane (top surface) is completely uniform [see Fig. 4(b1)].

Higher-order NLSMs can be realized by invoking the Wilsonian spin-density-wave (WSDW) mass orders, captured by the effective single-particle Hamiltonian

$$\hat{h}_{\text{WSDW}}^{\text{NL}} = N_1^2(\mathbf{k}) \left[\sum_{j=1}^3 \Delta_j \sigma_j \otimes N'_j(\mathbf{k}) \right]. \quad (7)$$

Three components of WSDW are chosen to be

$$\begin{aligned} N'_1(\mathbf{k}) &= \sin(k_x) \sin(k_y) \tau_3 \sim k_x k_y \tau_3 : B_{1u}, \\ N'_2(\mathbf{k}) &= [\cos(k_x) + \cos(k_y) - b'] \tau_3 \sim (k_\perp^2 - b') \tau_3 : A_{2u}, \\ N'_3(\mathbf{k}) &= [\cos(k_x) - \cos(k_y)] \tau_3 \sim (k_x^2 - k_y^2) \tau_3 : B_{2u}, \end{aligned} \quad (8)$$

where $k_\perp^2 = k_x^2 + k_y^2$. We expand $N'_j(\mathbf{k})$ around the center of the Brillouin zone, allowing us to classify the WSDW orders according to their transformation under the D_{4h} group. Notice that all WSDW orders vanish at $k_z = 0$, due to the appearance of $N_1^2(\mathbf{k})$ in $\hat{h}_{\text{WSDW}}^{\text{NL}}$ [see Eq. (7)]. Thus the bulk nodal loop residing in the $k_z = 0$ plane remains protected in the presence of any such order [46].

The B_{1u} WSDW order reduces the two-dimensional drumhead surface state (with $d_c = 1$) into a pair of one-dimensional arc states, given by $k_x = 0$ and $k_y = 0$ in the (k_x, k_y) plane [see Fig. 4(a2)]. Across these two specific directions the B_{1u} order changes its sign, and takes the profile of a domain wall mass. The corresponding LDOS in the xy plane reveals the underlying one-dimensional hinge modes (with $d_c = 2$) [see Fig. 4(b2)], realizing a second-order NLSM.

The subsequent addition of the A_{2u} WSDW order introduces a mass order for one-dimensional arc states of the second-order NLSM, with the profile of a domain wall.

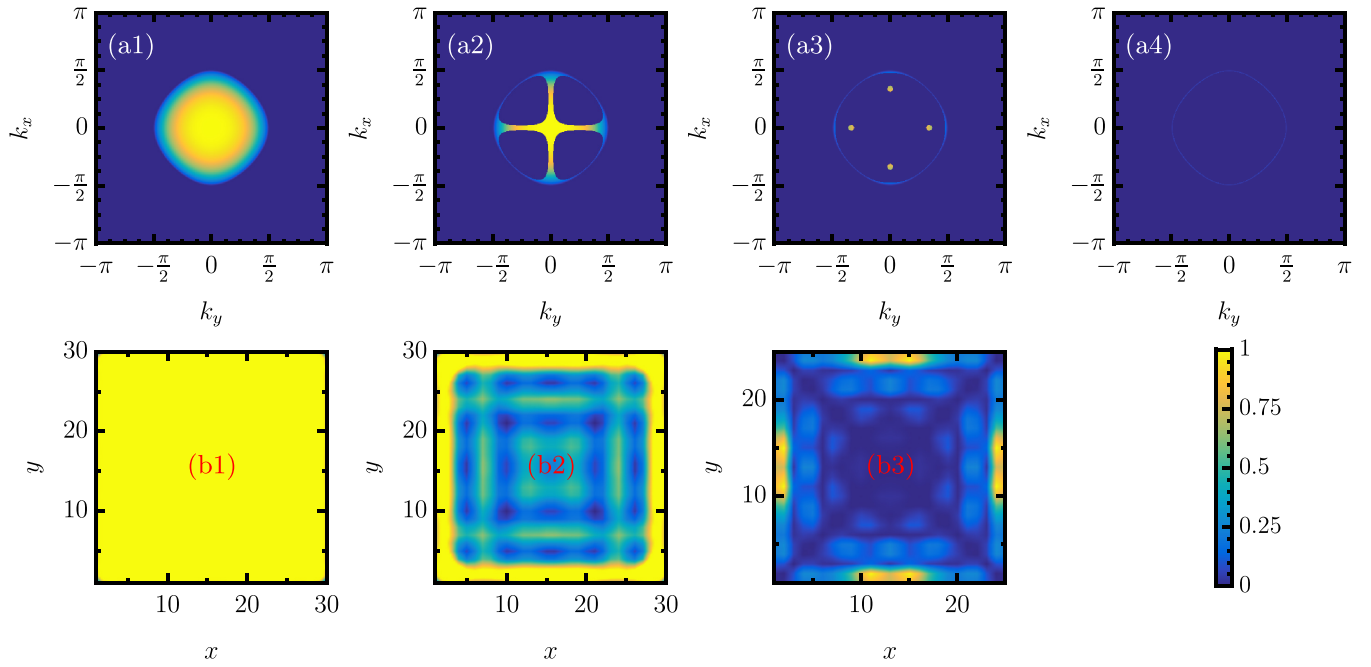


FIG. 4. Topologically protected surface modes for higher-order nodal-loop semimetals (NLSMs) in the reciprocal (top panel) and real (lower panel) space. Top panel: Square of the amplitude of near zero-energy states localized on the surface. Lower panel: Corresponding LDOS in real space [(b1) and (b2)] or amplitude of one of the near zero-energy states [for (b3)], with $E \sim 10^{-2}t$ (roughly). Here, (an), (bn) show the surface states for n th-order NLSM, for $n = 1, 2, 3$, and (a4) depicts absence of any localized surface states for a fourth-order NLSM. The faint peripheral states in (a2)–(a4) are the shadow of the delocalized states, connecting the top and bottom surfaces through the topologically protected bulk nodal loop. For numerical diagonalization we set $t = 1$, $b = 1$, $\Delta_1 = \Delta_2 = \Delta_3 = 0.3$, and $b' = 1.5$. The linear dimension in the z direction, along which we always implement an open boundary, is $L_z = 400$ (top panel), 10 [for (b1) and (b2)], and 25 [for (b3)] [46].

Specifically, this order changes sign when $\cos(k_j a) = b'$ for $j = x, y$. The surface states then undergo additional dimensional reduction and now support only four isolated zero-dimensional states in the (k_x, k_y) plane [see Fig. 4(a3)], when $b' > b$. The spatial distribution of one such state in the xy plane is shown in Fig. 4(b3), which takes the shape of zero-dimensional corner states (with $d_c = 3$), but now localized at the center of four edges. The resulting phase represents a third-order NLSM.

Finally, when we include B_{2u} WSDW order, the surface modes become completely gapped [see Fig. 4(a4)], and a fourth-order NLSM is realized. For all realizations of higher-order NLSMs the perimeter of the original drumhead surface state, accommodating delocalized states connecting the top and bottom surfaces through the bulk nodal loop, remains unaffected. In turn, this observation confirms that the WSDW orders (a) do not affect the bulk nodal loop, and (b) only cause dimensional reduction of the surface states, the quintessential features of any HOT phase of matter. The existence of the topologically protected bulk nodal loop for all higher-order NLSMs is further substantiated from the scaling of the density of states, namely, $g(E) \sim |E|$ in the bulk [46].

We note that it is also conceivable to realize a second-order NLSM in the presence of a Wilsonian charge density

wave, obtained by taking $\sigma_j N'_j(\mathbf{k}) \rightarrow \sigma_0 N'_1(\mathbf{k})$ in Eq. (7). The resulting arc states in the momentum space and the hinge modes in the real space are similar to the ones shown in Figs. 4(a2) and 4(b2), respectively, but we cannot proceed through the hierarchy of HOSMs any further with the charge-density-wave order.

To summarize, we here present a general principle for constructing HOT phases, including gapped [46] and gapless representatives. In particular, we illustrate the higher-order generalization of a topological Kondo insulator (see Fig. 1), TDSMs (see Figs. 2 and 3), which can be realized in Cd_3As_2 [51], Na_3Bi [52], and a NLSM (see Fig. 4), relevant for Ca_3P_2 [53], when subjected to lattice deformations thereby reducing the symmetry. This construction can also be applied to gapless superconductors, where the zero-energy modes residing on a surface of codimension $d_c = n$ are constituted by Majorana fermions. In particular, localized Majorana zero modes in the form of corner states can be useful for topological quantum computations [54].

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