

Universal higher-order topology from a five-dimensional Weyl semimetal: Edge topology, edge Hamiltonian, and a nested Wilson loop

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Higher-order topological insulators (HOTIs) or multipole insulators, hosting peculiar corner states, were discovered [Benalcazar *et al.*, *Science* **357**, 61 (2017) and Schindler *et al.*, *Sci. Adv.* **4**, eaat0346 (2018)]. It was independently discovered [Hashimoto *et al.*, *Phys. Rev. B* **95**, 165443 (2017)] that continuum five-dimensional (5D) Weyl semimetals generically host the corner states, and so do four-dimensional (4D) class A and three-dimensional (3D) class AIII topological insulators. In this paper we further confirm that the 5D Weyl semimetals, upon dimensional reduction, lead to universal higher-order topology. First we explain a discrete symmetry protecting the 5D Weyl semimetals, and describe dimensional reductions of the 5D Weyl semimetals to the popular HOTIs in the continuum limit. We calculate the topological charge carried by edge states of the 5D Weyl semimetal, for the most generic boundary condition. The topological charge is a Dirac monopole, which can also be seen from that edge Hamiltonians, are always of the form of a 3D Weyl semimetal. This edge topology leads to the edge-of-edge states, or the corner states, generically, suggesting that the 5D Weyl semimetal is thought of as a physical structural origin of corner states in HOTIs. In addition, we explicitly calculate a nested Wilson loop of the 5D Weyl semimetal and find that the topological structure is identical to that of a Wilson loop of a Dirac monopole.

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I. INTRODUCTION

Among various topological phases of matter, recently higher-order topology in condensed matter physics attracted attention, due to its peculiarity in dimensional aspects. Gapless states can show up not on the surface of materials but on corners or hinges, thus localized states as a result of the bulk topology has a spatial support whose dimensions are lower by two or more, compared to the bulk dimensions. The higher-order topology goes beyond the ordinary bulk-edge correspondence [1–3], thus any universal theoretical understanding of the higher-order topology is in demand.

Higher order topological insulators (HOTI) were introduced in seminal papers [4,5] (see for earlier related proposals [6,7], and a mathematical proposal [8]). The notion and mechanism of corner states were independently introduced in Ref. [9] (see also [10]), where a 5D Weyl semimetal was shown to host the corner states quite generically.

The Weyl semimetals [11] have particularly simple topological structures, and their higher dimensional generalization and its edge states were studied [12]. It was discovered in Ref. [13] that an edge state of the continuum 5D Weyl semimetal has a nontrivial topological charge, through an analogy of Nahm construction of monopoles [14] and a superstring T-duality. This observation lead to the notion of corner states in Ref. [9], since the topological charge of the edge state

means the existence of a corner state. The corner state was called in Ref. [9] as an “edge-of-edge state.”

In this paper we bridge the description of the corner states obtained in the 5D Weyl semimetals [9] and that of the popular HOTIs [4,5]. We first show that the popular HOTIs in the continuum are obtained by dimensional reduction of the 5D Weyl semimetal, and identify the discrete symmetry of the 5D Weyl semimetals. We explicitly describe the edge Hamiltonian and the edge topological charge of the 5D Weyl semimetal with a completely generic boundary condition, to show that the edge hosts a nontrivial topology of the form of a Dirac monopole. As for the generic boundary condition we follow the strategy developed in Ref. [15] for continuum Weyl semimetals. As HOTIs are often characterized by nested Wilson loops [4] and entanglement polarization [16], we explicitly calculate the nested Wilson loop of the 5D Weyl semimetals, to confirm that it is governed by a topology of a Dirac monopole. Therefore, in total, the higher order topology of the 5D Weyl semimetals is due to the common Dirac monopole structure in all of the following aspects: (1) edge Hamiltonian, (2) topology of the edge state, and (3) nested Wilson loop Hamiltonian.

This topological structure governed by the 5D Weyl semimetals can be identified in various recent studies of the higher-order topology. For example, topological quadrupole semimetals [17] host a topological semimetal structure on their surfaces, and the 5D Weyl semimetal shares [9] the same surface semimetal structure [18]. From these observations, we claim that, following [9], the 5D Weyl semimetal is a universal origin of the higher-order topology. Namely, for a class of microscopic Hamiltonians whose continuum limit is that of the continuum 5D Weyl semimetal (or a dimensional

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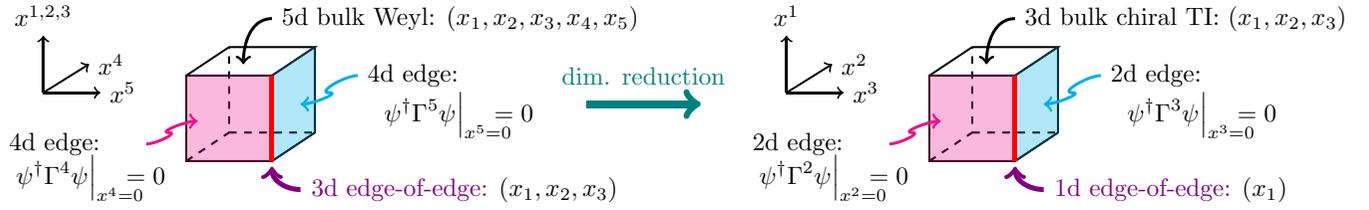


FIG. 1. The schematic picture of the corner state and the dimensional reduction from the 5D Weyl semimetal to the 3D chiral topological insulator (class AIII), taken from Fig. 1. of [9].

reduction of it), we claim that universally an edge-of-edge state appears.

The organization of this paper is as follows. In Sec. II we briefly review the corner states in the continuum 5D Weyl semimetals, with the most generic boundary conditions, obtained in Ref. [9]. In Sec. III we provide a relation between the popular HOTIs in the continuum and the 5D Weyl semimetals. In Sec. IV the effective Hamiltonian of the edge state is shown to be identical to that of a 3D Weyl. In Sec. V the topological charge carried by the most generic edge state of the 5D Weyl is shown to be that of a Dirac monopole. Then in Sec. VI we explicitly calculate the nested Wilson loop of the 5D Weyl semimetal and show that it is dictated by a monopole topological charge. The last section is for a summary and discussions. Appendix A is a proof of the most generic boundary condition of the 5D Weyl semimetal. Appendix B describes cases where corner states are absent in spite of the nontrivial topology.

II. REVIEW OF CORNER STATES IN 5D WEYL SEMIMETAL

In this section we give a review of generic corner (hinge) states in 5D Weyl semimetals, 4D class A and 3D class AIII topological insulators, obtained in Ref. [9]. The discovery of corner states [9] was independent of the discovery of multipole insulators [4]. The corner states are called edge-of-edge states in Ref. [9], but in this paper we call them corner states [19]. See Fig. 1 (taken from [9]) for the schematic view of the edge-of-edge states.

The Hamiltonian of the 5D Weyl semimetal [12] in the continuum limit is given by

$$H = \sum_{I=1}^5 p_I \Gamma_I, \quad (1)$$

where (p_1, \dots, p_5) is the momentum in the 5D space, and Γ_I is the 4×4 Γ matrices satisfying the Clifford algebra, $\{\Gamma_I, \Gamma_J\} = 2\delta_{IJ}$. It is the simplest to take the chiral representation of the Γ matrices,

$$\begin{aligned} \Gamma_i &\equiv \begin{pmatrix} 0 & -i\sigma_i \\ i\sigma_i & 0 \end{pmatrix} \quad (i = 1, 2, 3), \\ \Gamma_4 &\equiv \begin{pmatrix} 0 & \mathbf{1}_2 \\ \mathbf{1}_2 & 0 \end{pmatrix}, \quad \Gamma_5 \equiv \begin{pmatrix} \mathbf{1}_2 & 0 \\ 0 & -\mathbf{1}_2 \end{pmatrix}. \end{aligned} \quad (2)$$

Here $\sigma_i (i = 1, 2, 3)$ is the Pauli matrix. The 4D class A topological insulator is obtained by putting $p_5 = m_5$

(constant) [20]:

$$H_{4DA} = \sum_{i=1}^3 p_i \Gamma_i + p_4 \Gamma_4 + m_5 \Gamma_5. \quad (3)$$

The 3D class AIII topological insulator is a dimensional reduction $p_4 = m$ and $p_5 = 0$,

$$H_{3DAIII} = \sum_{i=1}^3 p_i \Gamma_i + m \Gamma_4. \quad (4)$$

The edge states of the 5D Weyl semimetals were studied in Ref. [12].

It was argued in Ref. [9] that the most general boundary condition at $x_5 = 0$, allowed by the Hermiticity of the system, is

$$(\mathbf{1}_2, -U_5^\dagger) \psi |_{x_5=0} = 0. \quad (5)$$

Here U_5 is a generic $U(2)$ constant matrix. We will provide a rigorous proof of this in Appendix A. Even under a dimensional reduction to HOTI or other topological insulators, this generic boundary condition (5) is not modified. Of course the dimensional reduction should not be made along the direction perpendicular to the introduced surface (which is x_5 in the example above). Note that this boundary condition is the most general one which respects the Hermiticity of the system with the Hamiltonian (1) in the continuum limit. The genericity means that any microscopic boundary condition at $x_5 = 0$ which does not break the Hermiticity should reduce to a certain U_5 if the Hamiltonian in the continuum limit is given by (1). Reverse engineering of finding a lattice boundary condition from a given U_5 is a nontrivial problem.

For surfaces not in $x_5 = 0$, one just makes a rotation in the 5D space together with the Γ matrices. For example, a surface at $x_4 = 0$ allows the following generic boundary condition [9]:

$$\left(\frac{1}{2}(U_4^\dagger - U_4), \mathbf{1}_2 - \frac{1}{2}(U_4 + U_4^\dagger) \right) \psi |_{x_4=0} = 0. \quad (6)$$

Here, again, U_4 is a general constant $U(2)$ matrix.

In Ref. [9] it was shown that in a 5D Weyl semimetal (1) with two surfaces with most generic boundary conditions (5) and (6), there exists generically a corner state localized at $x_4 = x_5 = 0$, with an energy ϵ given by a solution of the equation

$$A\epsilon^2 - 2B\epsilon + C = 0, \quad (7)$$

where

$$\begin{aligned} A &\equiv 1 - \cos^2 \theta_4 \cos^2 \theta_5, \\ B &\equiv a_i p_i \cos \theta_5 \sin^2 \theta_4 + b_i p_i \cos \theta_4 \sin^2 \theta_5, \\ C &\equiv (a_i p_i)^2 \sin^2 \theta_4 + (b_i p_i)^2 \sin^2 \theta_5 - p_i^2 \sin^2 \theta_5 \sin^2 \theta_4. \end{aligned} \quad (8)$$

In this expression we have parametrized the boundary condition parameters U_5 and U_4 as

$$U_5 \equiv e^{i\theta_5}(a_0\mathbf{1}_2 + ia_i\sigma_i), \quad U_4 \equiv e^{i\theta_4}(b_0\mathbf{1}_2 + ib_i\sigma_i), \quad (9)$$

with $a_0^2 + a_i^2 = b_0^2 + b_i^2 = 1$.

The simplest example presented in Ref. [9] was a corner state with a dispersion $\epsilon = -p_1$, with the following boundary conditions at the intersecting surfaces:

$$(\Gamma_4 - i\Gamma_3)\psi|_{x_4=0} = 0, \quad (\Gamma_5 - i\Gamma_2)\psi|_{x_5=0} = 0. \quad (10)$$

Another simple example in a class AIII topological insulator (4) was given in Ref. [9] as a localized state at the corner $x_2 = x_3 = 0$ with a dispersion $\epsilon = -p_1$ with the following boundary conditions:

$$(\Gamma_2 - i\Gamma_5)\psi|_{x_2=0} = 0, \quad (\Gamma_3 - i\Gamma_4)\psi|_{x_3=0} = 0. \quad (11)$$

The 5D Weyl semimetal (1) has a topological defect centered at $p_I = 0$ from which a 1-form flux $*(F \wedge F)$ made of the second Chern class density emanates. This can be easily confirmed by the dimensional reduction to the 4D topological insulator of class A (3). the bulk topology is the second Chern class of the Berry connection [21],

$$\frac{1}{16\pi^2} \int dp_1 dp_2 dp_3 dp_4 \text{tr}[F_{\mu\nu} * F_{\mu\nu}] = -\frac{1}{2} \text{sgn}(m_5). \quad (12)$$

The dimensional reduction corresponds to taking a slice of the originally 5D momentum space, so the reduced system inherits partly the original topological structure.

Introducing a surface was interpreted as a T-duality in string theory [13], and because of that, the edge state on the surface of the 4D class A system was shown to have an independent topological charge [13]. It leads to a prediction of having a corner (hinge) state once another surface is introduced to the system. As a result, various corner (hinge) states were constructed in Ref. [9].

III. 5D WEYL AND HOTI

In this section we study the genericity of our 5D Weyl Hamiltonian, in particular in regards to HOTIs. We specify the discrete symmetry which brings any four-band system to 5D Weyl semimetals. If we regard some of the components of the 5-momentum p_I as a constant or zero, then this system reduces to lower-dimensional semimetals/insulators. We describe dimensional reduction to two popular examples of higher-order topological insulators provided in Refs. [4,5].

First, let us point out an important discrete symmetry which protects the Weyl Hamiltonian (1). Suppose we are interested in four-band material, then the Hamiltonian is a four-by-four Hermitian matrix. Any such matrix H can be expanded as

$$H = p_0\mathbf{1}_4 + \sum_{I=1}^5 p_I \Gamma_I + i \sum_{I>J} p_{IJ} \Gamma_I \Gamma_J. \quad (13)$$

Here p_0 , p_I , and p_{IJ} are real parameters.

In even dimensions $D = 2n$, the 2^n -dimensional representation of Clifford algebra is known to be unique, so the representation Γ_I ($I = 1, \dots, 2n$) should be related to its transpose $(\Gamma_I)^T$ by a similarity transformation $C\Gamma_I C^{-1} = c(\Gamma_I)^T$, with

a constant $c = \pm 1$. Our five-dimensional Γ matrices are obtained by adding Γ_5 , which is given by a product $\Gamma_1\Gamma_2\Gamma_3\Gamma_4$ up to a sign, to the $D = 4$ case, so Γ_5 is subject to the same similarity transformation, and c is known to be equal to 1.

Suppose we impose the invariance of the matrix H (13) under the similarity transformation C ,

$$CHC^{-1} = (H)^T. \quad (14)$$

Then we find that the last term $\Gamma_I\Gamma_J$ is not invariant under this transformation, thus the symmetric Hamiltonian under C transformation is

$$H = p_0\mathbf{1}_4 + \sum_{I=1}^5 p_I \Gamma_I. \quad (15)$$

This is the Weyl Hamiltonian (1), as the first term $\mathbf{1}_4$ is a trivial addition to determine the zero of the whole energy spectrum. So we conclude that the similarity transformation C brings the general four-band system to the 5D Weyl semimetal. The resultant symmetric system has only five constant parameters, p_I ($I = 1, 2, 3, 4, 5$).

The physical understanding of the similarity transformation (14) is as follows. Our Γ matrices are Hermitian, so we may replace (14) by

$$CHC^{-1} = H^*. \quad (16)$$

This is known to be the PT symmetry (parity and time reversal symmetry) [22] if we regard the coefficients p_I , p_{IJ} do not change under the symmetry. In fact, if the coefficients are purely written by momenta, since the PT symmetry leaves momenta invariant, the coefficients are invariant. So in general the PT symmetry is our similarity transformation C .

The importance of the PT symmetry to restrict the structure of the four-band material is well known [23], in particular for classifying Dirac semimetals. Dirac semimetals in the continuum limit is a particular dimensional reduction of the 5D Weyl semimetal. Very recently, it was reported [24] that some Dirac semimetals host a higher-order topology, which is along our claim that the 5D Weyl semimetal is a universal origin of a class of the higher-order topology.

As a consequence of the similarity C , the resultant spectra is doubly degenerate. This is a consequence of the Kramers degeneracy in terms of the PT symmetry. As we will see in later sections, the degeneracy makes the Berry connection to be non-Abelian, and the non-Abelian structure is necessary for the system to host higher-order topology [25].

Now, let us describe two popular examples of HOTI [4,5] and show that these are dimensional reduction of 5D Weyl semimetals.

The first example is the famous 2D quadrupole insulator given by Benalcazar *et al.* [4]. It has a lattice Hamiltonian

$$H = -\sin k_x \Gamma_3 + (-1 + m_x + \cos k_x) \Gamma_4 - \sin k_y \Gamma_1 - (-1 + m_y + \cos k_y) \Gamma_2, \quad (17)$$

where (k_x, k_y) is the 2D momentum and m_x, m_y are nonzero constants. The expansion around $k_x, k_y, m_x, m_y \sim 0$ provides a continuum limit,

$$H_{\text{HOTI}} = (-k_y) \Gamma_1 + (-m_y) \Gamma_2 + (-k_x) \Gamma_3 + m_x \Gamma_4. \quad (18)$$

This system hosts a corner state [4]. The identification with the 5D Weyl semimetal is obvious,

$$\begin{aligned} p_1 &= -k_y, & p_2 &= -m_y, & p_3 &= -k_x, \\ p_4 &= m_x, & p_5 &= 0. \end{aligned} \quad (19)$$

So the x direction in Ref. [4] is the $(-x_3)$ direction, and the y direction in Ref. [4] is the $(-x_1)$ direction. This identification is made explicit to match the notation of [4], but identification with any $SO(5)$ -rotated frame leads to the same physical spectra. In Ref. [4] the boundary conditions at the two orthogonally intersecting edges were derived (see the supplement Sec. II of [4]), and in our notation they are

$$(\mathbf{1}_4 - i\Gamma_3\Gamma_4)\psi|_{x_3=0} = 0, \quad (\mathbf{1}_4 + i\Gamma_1\Gamma_2)\psi|_{x_1=0} = 0. \quad (20)$$

These boundary conditions turn out to be identical to the ones (10) given in Ref. [9]. In fact, if we make the following renaming of coordinates:

$$(x_1, x_2, x_3, x_4, x_5) \rightarrow (x_5, x_2, x_4, x_3, -x_1), \quad (21)$$

this brings (10) to (20).

Another popular example of the higher-order topological insulator was given by Schindler *et al.* in Ref. [5], a 3D insulator with $C_4^z T$ symmetry,

$$\begin{aligned} H &= \left(2 + \sum_i \cos k_i\right) \Gamma_5 + \sum_i \sin k_i \Gamma_i \\ &+ \Delta_2(\cos k_x - \cos k_y) \Gamma_4. \end{aligned} \quad (22)$$

Expanding this lattice Hamiltonian around the band inversion point $k_i = (\pi, \pi, \pi)_i + \tilde{k}_i$, a continuum Hamiltonian is obtained as

$$H = \sum_i \tilde{k}_i \Gamma_i - \Gamma_5. \quad (23)$$

This can be interpreted as the 3D class AIII Hamiltonian (4) under swapping Γ_4 and Γ_5 , so it is given by a dimensional reduction from the 5D Weyl semimetal. The result of [5] showing the hinge states is consistent with [9] claiming general hinge states for the class AIII topological insulators. It should be noted here also that the HOTI (18) is a trivial dimensional reduction of a 3D class AIII topological insulator (4).

Note that all known examples of HOTI use Hamiltonians with at least four bands [26]. It was shown in Ref. [9] that 3D Weyl semimetals cannot host a corner state, meaning that two-band Hamiltonian cannot be a HOTI. From the generic behavior of the 5D Weyl semimetal hosting corner states, we may argue that among all possible four-band Hamiltonians the structure of the Γ matrices is important to host the corner states. A physical reason for this is the edge topological charge [13], derived through an analogy to the Nahm construction of monopoles and string T-duality.

IV. EDGE HAMILTONIAN

In this section we calculate the edge Hamiltonian for edge states in the 5D Weyl semimetal with the generic boundary condition (5). We show explicitly that the edge Hamiltonian has the structure of a 3D Weyl semimetal.

For the general boundary condition (5), the edge state wave function is expressed as [9]

$$\psi = \begin{pmatrix} \mathbf{1}_2 \\ U \end{pmatrix} \xi \exp[ip_L x']. \quad (24)$$

The edge state is given by (24), and if we choose the basis 2-spinor as $\xi_1 = (1, 0)^T$ and $\xi_2 = (0, 1)^T$, then these ξ_a ($a = 1, 2$) give the following basis for the 4-spinor:

$$\psi_a \equiv \begin{pmatrix} \mathbf{1}_2 \\ U \end{pmatrix} \xi_a. \quad (25)$$

Using this, the effective Hamiltonian for the edge states,

$$H_{ab}^{(\text{eff})} \equiv \int d^5x \psi_a^\dagger H \psi_b, \quad (26)$$

is calculated as

$$H^{(\text{eff})} = \cos \theta \tilde{p}_4 \mathbf{1}_2 + \sin \theta \tilde{p}_i \sigma_i, \quad (27)$$

where we decomposed the $U(2)$ matrix to a product of a $U(1)$ phase θ and an $SU(2)$ matrix U' ,

$$U = e^{i\theta} U' \quad (28)$$

and we defined the $SO(4)$ rotated momentum frame $(\tilde{p}_i, \tilde{p}_4)$ by the following $SU(2)$ matrix relation:

$$(-ip_i \sigma_i + p_4) U' = -i\tilde{p}_i \sigma_i + \tilde{p}_4. \quad (29)$$

This edge Hamiltonian $H^{(\text{eff})}$ (27) is of the form of a 3D Weyl semimetal, so the edge state is topological. Therefore, when another surface perpendicular to the original surface $x^5 = 0$ is introduced, a corner state is expected to exist at the intersection of the surfaces, due to the topological structure of the edge Hamiltonian.

Note that this argument is to present a general framework of the emergence of the corner states. Whether the corner state actually exists or not in a particular given setup depends on more details of the system. There are at least two reasons for this. First, if the effective Hamiltonian (27) is that of a 3D type II Weyl semimetal [27], because the existence of an edge state for a given type II Weyl semimetal depends on the surface direction [28], our 5D system may not give a corner state. Second, it is possible that the 3D Weyl Hamiltonian structure may be accidentally inactive for particular dimensional reductions to realistic dimensions. For example, if the directions \tilde{p}_i in Eq. (27) are all dimensionally reduced, the Hamiltonian simply reduces to a unit matrix which does not have any topological structure. Concerning the first reason, we describe a concrete example in Appendix B.

We will calculate the topological charge in the next section. For the calculation we need the wave function which is defined by ξ . The effective Hamiltonian is diagonalized by a solution of

$$(\pm \sqrt{\tilde{p}_i^2} \mathbf{1}_2 - \tilde{p}_i \sigma_i) \xi = 0. \quad (30)$$

The energy ϵ is given by

$$\epsilon = \tilde{p}_4 \cos \theta \pm \sqrt{\tilde{p}_i^2} \sin \theta, \quad (31)$$

which is consistent with the result in Ref. [9].

In obtaining the effective Hamiltonian, we did not include the x_5 dependence in the wave function (25). It is not a problem, because the relevant term disappears when evaluating the effective Hamiltonian, due to the Hermiticity condition (A6). In order to extract the information about x_5 dependence from this effective Hamiltonian approach, we instead consider the following equation:

$$H\psi_a = E_a\psi_a + \sum_{b=1,2} \beta_{ab}\tilde{\psi}_b, \quad (32)$$

where $\tilde{\psi}_b$ ($b = 1, 2$) is the basis 4-spinor spanning the space orthogonal to the edge state space spanned by ψ_a ,

$$\tilde{\psi}_a = \begin{pmatrix} \mathbf{1}_2 \\ -U \end{pmatrix} \xi_a \exp[ip_I x^I]. \quad (33)$$

For Eq. (32) to be a Hamiltonian eigenequation for the edge state, we need to require $\beta_{ab} = 0$. Since β is given by

$$\beta_{ba} = \int d^5x \tilde{\psi}_b^\dagger H \psi_a, \quad (34)$$

we can calculate it explicitly as

$$\begin{aligned} \beta &= \begin{pmatrix} \mathbf{1}_2 \\ -U \end{pmatrix}^\dagger H \begin{pmatrix} \mathbf{1}_2 \\ U \end{pmatrix} \\ &= p_5 \mathbf{1}_2 + i(\sin \theta \tilde{p}_4 \mathbf{1}_2 - \cos \theta \tilde{p}_i \sigma_i). \end{aligned} \quad (35)$$

Because the eigenvalue of this expression needs to vanish, we find that the momentum p_5 has to be pure imaginary and is given by

$$p_5 = i\alpha \equiv -i(\sin \theta \tilde{p}_4 \mp \cos \theta \sqrt{\tilde{p}_i^2}). \quad (36)$$

The signs are for the two edge states, respectively. The edge states are localized at the surface $x_5 = 0$, thus the wave function should have a pure imaginary momentum p_5 . The normalizability of the wave function restricts the possible momentum region of (p_i, p_4) for the existence of the edge state.

V. EDGE TOPOLOGICAL CHARGE

In this section we show that the topological charge of the generic edge state of the 5D Weyl semimetal is a Dirac monopole. As we described in the Introduction, the corner states in the 5D Weyl semimetals are a consequence of the topological charge of the edge states. In Ref. [13], for a particular boundary condition of a 4D class A topological insulator, the edge state is shown to carry a topological charge of a Dirac/non-Abelian monopole. It was argued in Ref. [9] that the edge topological charge can be generally the same for the 5D Weyl semimetals. Here we explicitly confirm it, by providing the topological charge of the edge state of the 5D Weyl semimetal (1) with arbitrary boundary condition (5).

Let us calculate the topological charge of the edge state. It was shown in Ref. [9] that the edge state has a topological charge which is the same type as that of the 3D Weyl semimetal. Here we demonstrate it explicitly. For a particular choice of the boundary condition, the topological charge was calculated in Ref. [13].

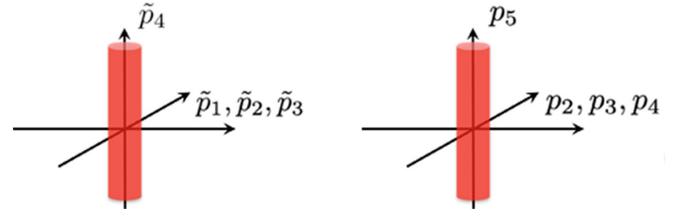


FIG. 2. The structure of the topological charges. Left: The topological charge distribution of the edge state. It is a Dirac monopole situated at the origin of $\tilde{p}_1, \tilde{p}_2, \tilde{p}_3$ space. They are aligned along the \tilde{p}_4 direction, so it is a monopole string. The 4-momentum $\tilde{p}_1, \dots, \tilde{p}_4$ is rotated from the original 4-momentum, p_1, \dots, p_4 for the edge at $x_5 = 0$, and \tilde{p}_4 direction in the original momentum space depends on the boundary condition. Right: The topological charge of the Hamiltonian H_1 of the nested Wilson loop along p_1 , given in Eq. (57). The Dirac monopole is located at the origin of p_2, p_3, p_4 space. It has no dependence in p_5 , so the monopole string extends along the p_5 axis. The direction of the monopole string depend on the gauge condition of the original 5D Berry connection, but independent of the gauge condition for the Berry connection for H_1 .

As we have seen in the previous section, the effective Hamiltonian for edge states is diagonalized by solutions of (30). We name the two solutions of (30) as ξ_+ and ξ_- depending on the \pm sign in Eq. (30). As they can be regarded as the energy eigenstates of a 3D Weyl semimetal Hamiltonian (27), it naturally leads us to suggest that the edge state has a topological charge. In fact, we can calculate the Berry connection associated with ξ_+ and show that it is the connection for a Dirac monopole,

$$\tilde{A}_1 + i\tilde{A}_2 = \frac{i(\tilde{p}_1 + i\tilde{p}_2)}{2\sqrt{\tilde{p}_i^2}(\sqrt{\tilde{p}_i^2} - \tilde{p}_3)}, \quad \tilde{A}_3 = \tilde{A}_4 = 0. \quad (37)$$

Here \tilde{A} is the connection in the rotated frame spanned by $(\tilde{p}_i, \tilde{p}_4)$. It is defined by [29]

$$\tilde{A}_i = \int d^5x i\psi^\dagger \frac{d}{d\tilde{p}_i} \psi, \quad \tilde{A}_4 = \int d^5x i\psi^\dagger \frac{d}{d\tilde{p}_4} \psi. \quad (38)$$

The Dirac monopole (37) sits at the origin of (\tilde{p}_i) ($i = 1, 2, 3$) space, and it extends to the \tilde{p}_4 direction. So this is a monopole string in the 4D momentum space. The location of the monopole string is at $\tilde{p}_i = 0$. (Note that the ‘‘string’’ of the ‘‘monopole string’’ is different from the Dirac string associated with a three-dimensional monopole; the former is physically extending along the \tilde{p}_4 direction while the latter is a gauge artifact.) See Fig. 2 (left) for the configuration of the monopole string.

If we go back to the original momentum space spanned by (p_i, p_4) , this monopole string is also rotated back. The direction of the extension of the monopole string is specified by a straight line

$$\text{tr}[\sigma_j(-ip_i\sigma_i + p_4)U'] = 0 \quad (j = 1, 2, 3). \quad (39)$$

Let us study how the topological charge looks like after the dimensional reduction to the HOTI (18). In the notation above, the surface is introduced at $x_5 = 0$, so the reduction to (18) means placing three of the other momenta by some

constant, for example,

$$p_2 = m_x, \quad p_3 = m_y, \quad p_4 = 0. \quad (40)$$

Upon this reduction we have a 2D system spanned by p_1 and p_5 . The edge topological charge is seen only as a slice (40) of the monopole string. Only possible index associated with the edge state of the dimensionally reduced system is the Wilson loop,

$$W \equiv \int_{-\infty}^{\infty} dp_1 A_1, \quad (41)$$

since the valid quantum number of the edge state is only p_1 . This W is defined as an integral over the slice. It is easy to see that this quantity is generically nonzero, due to the monopole string in the higher-dimensional momentum space. However, the value of W is not quantized, and it depends on the parameters m_x , m_y , and U . In particular, it depends on the angle between the edge momentum direction (the p_1 axis) and the plane spanned by the \tilde{p}_4 axis and the \tilde{p}_3 axis. When they are parallel to each other, W vanishes, due to the vanishing components of (37). This complication always emerge after dimensional reductions, because the topological charge defined in the higher dimensional momentum space can never be captured naturally just by looking at the connections on the slices.

VI. NESTED WILSON LOOP

So far we have presented the topological structure of the most generic edge states of the continuum 5D Weyl semimetal. On the other hand, it was shown that the nested Wilson loop [4] captures the topological property of HOTIs [30], so here we explicitly calculate the nested Wilson loop for the continuum 5D Weyl semimetal. We show that the nested Wilson loop is identical to a Wilson loop in a 4D momentum space with a Dirac monopole string.

First we obtain the normalized energy eigenstates of the bulk Hamiltonian (1). The energy eigenvalues are $\pm p$ with $p \equiv \sqrt{p_7^2}$, and we take the positive energy eigenstates. The degenerate two eigenstates are aligned together to form a 4×2 matrix Ψ satisfying $H\Psi = p\Psi$,

$$\Psi = \sqrt{\frac{p-p_5}{2p}} \begin{pmatrix} \mathbf{1}_2 \\ F \end{pmatrix}, \quad (42)$$

where

$$F \equiv \frac{1}{p_5 - p} (p_4 \mathbf{1}_2 + i p_i \sigma_i). \quad (43)$$

With this energy eigenstate, the Berry connection

$$A_I \equiv i\Psi^\dagger \frac{\partial}{\partial p_I} \Psi \quad (44)$$

can be calculated explicitly,

$$A_1 = C_A(p_4\sigma_1 + p_3\sigma_2 - p_2\sigma_3), \quad (45)$$

$$A_2 = C_A(p_3\sigma_1 - p_4\sigma_2 + p_1\sigma_3), \quad (46)$$

$$A_3 = C_A(-p_2\sigma_1 - p_1\sigma_2 - p_4\sigma_3), \quad (47)$$

$$A_4 = C_A(-p_1\sigma_1 + p_2\sigma_2 + p_3\sigma_3), \quad (48)$$

$$A_5 = 0, \quad (49)$$

with an overall common coefficient $C_A \equiv 1/[2p(p+p_5)]$.

Let us calculate the Wilson loop (line) of the Berry connection along the p_1 direction,

$$W_1 \equiv \text{P exp} \left[i \int_{-\infty}^{\infty} A_1 dp_1 \right], \quad (50)$$

where ‘‘P’’ means a path ordering which makes W gauge covariant. We diagonalize the Berry connection A_1 using a unitary matrix V_1 ,

$$A_1 = \lambda V_1^\dagger \sigma_3 V_1. \quad (51)$$

Here $\pm\lambda$ is the eigenvalue of A_1 ,

$$\lambda \equiv \frac{\sqrt{p_2^2 + p_3^2 + p_4^2}}{2p(p+p_5)}. \quad (52)$$

Since the unitary matrix V_1 does not depend on p_1 , the path ordering becomes trivial and we have

$$W_1 = V_1^\dagger \exp \left[i\sigma_3 \int_{-\infty}^{\infty} \lambda dp_1 \right] V_1. \quad (53)$$

The integral is evaluated explicitly and we obtain

$$W_1 = V_1^\dagger \begin{pmatrix} e^{is} & 0 \\ 0 & e^{-is} \end{pmatrix} V_1, \quad (54)$$

with [31]

$$s \equiv 2 \arctan \frac{\sqrt{p^2 - p_1^2 - p_5}}{\sqrt{p^2 - p_1^2 + p_5}}. \quad (55)$$

To evaluate the nested Wilson loop, we consider a Wilson loop Hamiltonian

$$H_1 \equiv -i \log W_1, \quad (56)$$

which is calculated as

$$H_1 = V_1^\dagger \sigma_3 V_1 s. \quad (57)$$

This H_1 is interpreted as some sort of the edge Hamiltonian for a 4D system on the edge at $x_1 = \text{const.}$ surface as it is obtained from the Wilson loop along the p_1 direction. This H_1 depends on the gauge condition, and in the present gauge, it is independent of p_5 apart from the overall factor s .

Now we consider the eigenstates of H_1 . Since the matrix part of this H_1 is proportional to A_1 itself, and it is of the form of a 3D Weyl semimetal, the Berry connection of the eigenstate of this H_1 is that of a Dirac monopole located at $p_2 = p_3 = p_4 = 0$. The monopole extends along p_5 , so, precisely speaking, the topological defect is a monopole string. The direction depends on the gauge condition of the 5D Berry connection (45)–(49), but independent of the gauge condition of the Berry connection of the eigenstate of H_1 . See Fig. 2 (right) for the configuration of the monopole string.

Therefore, the nested Wilson loop is identical to a Wilson loop of a Dirac monopole string. For example, a nested Wilson

loop along the p_4 direction at $p_2 = p_3 = -\infty$ is calculated as

$$W_4^{(1)} = \frac{\pi}{2}. \quad (58)$$

Here “ $W_4^{(1)}$ ” means the nested Wilson loop along p_4 obtained through the Wilson loop along p_1 .

It is easy to evaluate other nested Wilson loops $W_j^{(l)}$. All nested Wilson loops are nontrivial due to the topological structure of the monopole string, except for the ones involving the p_5 direction $l = 5$ (or $J = 5$). Since in our gauge condition the p_5 direction is special as the Berry connection vanishes there [see (49)], the nontrivial structure is hidden for Wilson loops associated with p_5 .

Note that the trivialization of the path ordering is not accidental; it is due to a careful choice of the gauge condition of the Berry connection, which originates in the choice of the basis of the eigenstates (42). In fact, we could have chosen some other set of basis of the degenerate eigenstates, for example (42) multiplied by some arbitrary $U(2)$ unitary matrix from the right, without losing the orthonormality. This matrix can depend on p_l , and this results in a gauge transformation of the Berry connection. So the choice of the gauge condition given by (42) makes the calculation of the Wilson loop possible [32].

It is amusing to point out that the calculation of the nested Wilson loop Hamiltonian H_1 is almost identical to what Atiyah and Manton did in 1989 [33], so-called Atiyah-Manton approach for skyrmions. The Hamiltonian H_1 corresponds to the pion field of the Skyrme model [34–36]. The wrapping number, which is the baryon number in the Skyrme model, is nontrivial when the pion field has the hedge-hog ansatz. This hedge-hog ansatz is nothing but the 3D Weyl semimetal Hamiltonian in condensed matter physics. In this analogy to make sense, we need to exchange x in the Skyrme model and p in condensed matter physics, with a careful check of the Berry connection (45)–(48) to completely coincide with a renowned BPST instanton [37], as demonstrated in Ref. [38].

We conclude that the nested Wilson loops of the 5D Weyl semimetal at the continuum are topologically nontrivial and the topological structure is that of a Wilson loop in a monopole string. $W_j^{(l)}$ ($l \neq 5$) is identical to a Wilson loop along p_l of a monopole string where the Dirac monopole center is located at $p_K = 0$ ($K \neq l$, $K \neq 5$).

This picture survives any dimensional reduction along the directions $\neq p_l$ and $\neq p_J$. In particular, the nested Wilson loop $W_2^{(1)}$ is of course identical with that evaluated in the quadrupole insulator [4] upon the dimensional reduction (19).

VII. SUMMARY AND DISCUSSION

In summary, we have bridged the higher-order topology of the 5D Weyl semimetals [9] and that of HOTIs, by showing that their Hamiltonians are related each other in the continuum. We have found that the 5D Weyl semimetal has the topological structure of the Dirac monopole from every aspect: the edge Hamiltonian (Sec. IV), the edge topological charge (Sec. V), the nested Wilson loop, and the entanglement polarization (Sec. VI). Therefore, the 5D Weyl semimetal can be regarded as a universal origin of a class of HOTIs. The 5D Weyl semimetal is obtained in the continuum limit of four

bands with two pairs of double degeneracy which is protected by the PT symmetry. Note that our argument is effective at the continuum limit where various crystalline symmetries disappear, so our universality refers to that of a universality class in the continuum limit or in the low-energy limit which is not protected by crystalline symmetries. As a scope of this work, this offers a novel criterion for how one can obtain HOTIs, due to its continuum structure.

We have described relations between the continuum 5D Weyl semimetals and the popular HOTI models. The corner states of the 5D Weyl semimetal, obtained in Ref. [9], are shown in various manners to lead to genetic HOTIs, as originally anticipated in Ref. [9]. We have explicitly calculated the topological charge of the edge state of the continuum 5D Weyl semimetal, with the most generic boundary condition on the surface, and have shown that it is a Dirac monopole (precisely, it is a monopole string in a 4D momentum space). The effective Hamiltonian of the edge state is shown to possess the structure of a 3D Weyl semimetal, which is consistent with the topological charge. These calculations generalize [13] and confirm the edge topological structure of [9], leading to the generic existence of the corner state. Furthermore, we have given the explicit calculation of the nested Wilson loop of the continuum 5D Weyl semimetal, and found that the topological structure is identical to that of a Wilson loop in the 4D momentum space with a Dirac monopole string. The 5D Weyl semimetals can be dimensionally reduced to the realistic HOTI models, while keeping the topological structure originated in the five dimensions. It is worth being emphasized that the three methods, the edge Hamiltonian, the edge topological charge, and the nested Wilson loop, do not require how the two surfaces intersect. Hence the universality is applied for intersection of surfaces at a generic angle.

Our study and [9] suggests that one of the bulk origins of generic corner states is the second Chern class. In fact, the edge topology which is the Dirac monopole is a consequence of the T-duality of the bulk Yang-Mills instanton hosting the second Chern class [13], and the bulk 5D Weyl semimetal has the second Chern class on the four-dimensional slice [38]. This structure may be hidden once a dimensional reduction to lower dimensions is made. However, since there exists a generic mechanism of the existence of the corner states due to the 5D Weyl semimetals, generically after the dimensional reduction the possibility of having the corner states remains.

To look back, the study [9] was motivated by elementary particle theories which are often in the continuum limit. Although a detailed study in condensed matter physics requires lattice Hamiltonians, which are lacking in Ref. [9], continuum limit generically provides a universal viewpoint which is irrelevant to detailed microscopic theories. Bridging particle physics and condensed matter physics has played quite an important role so far. In particle physics, it has been known for many years that the anomaly inflow argument [39] provides fermion modes localized at codimension two hypersurface (that is, a string in three spatial dimensions), and this is one historical origin of hinge states. Based on this, fermion localization at the intersection of surfaces in six dimensions was studied [40,41] for an application to 4D chiral gauge theories. Further symmetry/anomaly arguments may lead to various interesting researches bridging the particle

and condensed matter physics. In particular, particle physics is formulated to treat intrinsically many-body systems, and a quantum-field-theoretic definition of multipoles [42] may be of importance.

Some comments on possible future directions are in order. In this paper we concentrated on the second-order topological insulators and hinge states, and a generalization to third order (and higher) is important. To host the third order, one needs eight bands, so the instanton may be an octonionic instanton [43]. Some usage of higher-dimensional Clifford algebra [44,45] may help building the bridge. It is expected that on the surface of the eight-band system the BPST instanton emerges as the surface topological charge.

It should be noted that Weyl semimetals admit various deformations: the tilt of the Weyl cones, producing type II Weyl semimetals [27], as well as type III and type IV Weyl semimetals [46]. In particular, similarities to black hole spacetime was suggested [47], and its relevance to the surface state was studied [28]. The tilt of the edge dispersion can be interpreted [38] as a monopole in noncommutative space [48,49], and these ideas may be unified in higher dimensions of momenta. The localization of the fermions at corners may be affected by the deformation, as was reported for example in non-Hermitian deformations [50]. A deformation which breaks the PT symmetry was analyzed in Ref. [12], and it would be interesting whether the corner states may survive or not. Furthermore, the “deformation” going back to the microscopic Hamiltonian will necessarily introduce a Brillouin zone which suffers from the doubling of the Weyl points [51,52]. The continuum limit corresponds to a zoom-in on a small region around a Weyl point. As long as the Weyl points of the opposite signature are separated, our monopole-string structure will persist, and the corner state will survive. As well as these possible deformations, one should be careful in treating the dimensional reduction, as various dimensional reduction provides deformations which could change the topological properties. For example, a possible relation between the interpretation of HOTI as a piled-up Chern insulator [53] and our dimensional reduction needs to be clarified.

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APPENDIX A: GENERIC BOUNDARY CONDITION

It was studied in Ref. [9] that all possible boundary conditions of the continuum 5D Weyl semimetal (1) are parametrized by a $U(2)$ matrix (see [15] for the case of the 3D Weyl semimetal). Here we derive the same result in a more rigorous manner. We use this result in Secs. V and IV to evaluate the topological charge of the generic edge state and the effective edge Hamiltonian.

We put the boundary surface at $x^5 = 0$ without losing its generality. The boundary condition is of the form

$$M\psi|_{x^5=0} = 0, \quad (\text{A1})$$

where M is some constant matrix, and ψ is the wave function. Since this M has to have four linearly independent eigenvectors to constrain the whole wave function space, M is diagonalizable. And M has to project out half of the degrees of freedom of ψ at the boundary, so two of the four eigenvalues should be zero. Therefore, there exists a regular matrix B with which

$$M = B^{-1}DB, \quad D = \text{diag}(0, 0, a, b), \quad (\text{A2})$$

with $a, b \neq 0$. Decomposing ψ and B as their 2-spinor subspaces,

$$\psi|_{x^5=0} \equiv \begin{pmatrix} \xi \\ \eta \end{pmatrix}, \quad B = \begin{pmatrix} B_1 & B_2 \\ B_3 & B_4 \end{pmatrix}, \quad (\text{A3})$$

we can rephrase (A1) as

$$B_3\xi + B_4\eta = 0. \quad (\text{A4})$$

When $\det B_4 \neq 0$, we solve this as

$$\eta = -B_4^{-1}B_3\xi. \quad (\text{A5})$$

Next, we impose the boundary Hermiticity condition: for any ψ_i satisfying $M\psi_i = 0$, we need

$$\psi_i^\dagger \Gamma_5 \psi_j = 0. \quad (\text{A6})$$

The latter equation is equivalent to

$$\xi_1^\dagger \xi_2 = \eta_1^\dagger \eta_2. \quad (\text{A7})$$

substituting the solution (A5) of the boundary condition (A1) to this equation, we find

$$(B_4^{-1}B_3)^\dagger B_4^{-1}B_3 = \mathbf{1}_2, \quad (\text{A8})$$

as (A7) needs to be satisfied for arbitrary ψ satisfying the boundary condition (A1). This shows that $-B_4^{-1}B_3$ is a $U(2)$ unitary matrix U , so we derive the generic boundary condition

$$\eta = U\xi \quad (\text{A9})$$

for a $U(2)$ matrix U .

There remains the case of $\det B_4 = 0$. In fact, it is possible to show that with $\det B_4 = 0$ the condition (A7) cannot be met except for a trivial solution $\eta = 0$, as in the following. So $\det B_4 \neq 0$ is necessary for (A1) to be a consistent boundary condition.

When $\det B_4 = 0$ and $B_4 \neq 0$, we name the zero eigenvector as $\eta^{(0)}$. Choose a vector $\eta^{(1)}$ which is perpendicular to $\eta^{(0)}$, as $(\eta^{(0)})^\dagger \eta^{(1)} = 0$.

(1) If $\det B_3 \neq 0$, the vectors which satisfy the boundary condition (A4) is

$$\psi = \begin{pmatrix} 0 \\ \eta^{(0)} \end{pmatrix}, \quad \tilde{\psi} = \begin{pmatrix} B_3^{-1}B_4\eta^{(1)} \\ \eta^{(1)} \end{pmatrix}. \quad (\text{A10})$$

(2) If $\det B_3 = 0$ and $B_3 \neq 0$, choose the zero mode of B_3 as $\xi^{(0)}$, then we obtain the vectors satisfying (A4) as

$$\psi = \begin{pmatrix} 0 \\ \eta^{(0)} \end{pmatrix}, \quad \tilde{\psi} = \begin{pmatrix} \xi^{(0)} \\ 0 \end{pmatrix}. \quad (\text{A11})$$

If $B_4 = 0$, then use two zero modes to form a solution to (A4) as

$$\psi = \begin{pmatrix} 0 \\ \eta^{(0)} \end{pmatrix}, \quad \tilde{\psi} = \begin{pmatrix} 0 \\ \eta'^{(0)} \end{pmatrix}. \quad (\text{A12})$$

In all of these three cases, we construct generic vectors satisfying (A4) as

$$\psi_i \equiv a_i \psi + b_i \tilde{\psi}, \quad (\text{A13})$$

with arbitrary complex constants a_i, b_i . Then we substitute them to the Hermiticity condition (A6). It turns out that for all of these three cases, (A6) for arbitrary a_i and b_i leads to $\eta^{(0)} = 0$. Therefore there is no solution to the boundary condition when $\det B_4 = 0$.

APPENDIX B: HERMITICITY CONDITION FOR EDGE HAMILTONIAN

In order to have a corner state, the edge effective Hamiltonian (27) must obey the Hermiticity condition at the corner of the edge. However, for a certain boundary condition of the edge, the effective Hamiltonian (27) takes the form of that of the type II Weyl semimetals, and depending on the direction of the other edge it may not host any corner state. Here we will show the condition for which the 5D Weyl semimetal does not have the corner state.

We consider the corner at $x^4 = 0$ on the edge at $x^5 = 0$. The rotated momentum frame is defined by using an SU(2) matrix U' , which is expressed generically as

$$U' = \cos \phi \mathbf{1}_2 + i \sin \phi n_i \sigma_i, \quad (\text{B1})$$

where n_i is a unit vector, which can be taken as $n_i = (0, 0, 1)_i$ without loss of generality. Then, the edge Hamiltonian is

expressed as

$$H^{(\text{eff})} = \cos \theta (\cos \phi p_4 + \sin \phi p_3) + \sin \theta [\tilde{p}_1 \sigma_1 + \tilde{p}_2 \sigma_2 + (\cos \phi p_3 - \sin \phi p_4) \sigma_3], \quad (\text{B2})$$

where \tilde{p}_1 and \tilde{p}_2 are linear combinations of p_1 and p_2 . As the momentum p_4 acts on the wave function ψ as the derivative $-i\partial_4$, the Hermiticity condition requires the surface term at the boundary (the corner at $x^4 = 0$) vanish,

$$\psi_1^\dagger (\cos \theta \cos \phi \mathbf{1}_2 - \sin \theta \sin \phi \sigma_3) \psi_2 = 0. \quad (\text{B3})$$

This condition must be satisfied for arbitrary wave functions ψ_1 and ψ_2 which satisfy the boundary condition at the corner. For $\psi_1 = \psi_2 = (v_1, v_2)^T$, the condition gives

$$\cos \theta \cos \phi (|v_1|^2 + |v_2|^2) - \sin \theta \sin \phi (|v_1|^2 - |v_2|^2) = 0, \quad (\text{B4})$$

which has no solution for

$$|\tan \theta \tan \phi| < 1. \quad (\text{B5})$$

Therefore, for the boundary condition with (B5), the 5D Weyl semimetal has no corner state at $x^4 = x^5 = 0$.

The parameters θ and ϕ are the ones for the boundary condition at $x^5 = 0$. This means that one can even control the existence of the corner state by just modifying a boundary condition on a single surface. The corner state may become unstable under the adiabatic change of the boundary condition parameters of the surface. Here a peculiar interplay between the higher order topology and the type II Weyl semimetal is found.

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