Topological Inversion-Asymmetric Hinge States Protected by the Intrinsic Inversion Symmetry

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We propose inversion-asymmetric hinge states, which are different from the conventional inversion-symmetric hinge states in the higher-order topological insulators (HOTIs) realized in layered antiferromagnets (AFMs). First, we find all possible configurations of the hinge states in the HOTIs in all type-I magnetic space groups with inversion symmetry. In particular, in a layered AFM, we find a difference in the hinge states between the cases with an even and odd number of the layers. In the case of an even number of layers, which does not preserve inversion symmetry, positions of hinge states are not inversion symmetric. Nonetheless, these inversion-asymmetric hinge states result from the bulk topology protected by inversion symmetry. We show that their inversion-asymmetric configurations are uniquely determined from the symmetries and the topological invariant.

Introduction.—The discovery of topological insulators (TIs) have triggered intensive studies on topological aspects in electronic structures of solids [1, 2]. Three-dimensional (3D) TIs have gapless surface states which are protected by time-reversal (\(T\)) symmetry. On the other hand, these surface states can be gapped by breaking \(T\) symmetry while preserving topological properties of the bulk; such TIs are called magnetic TIs. Among magnetic TIs, those characterized by the quantized value of the Chern-Simons axion angle \(\theta = \pi [3–13]\) are known as axion insulators (AXIs). The simplest AXIs have been proposed in inversion (\(I\)) symmetric TIs in an external magnetic field and in a TI doped with magnetic atoms without breaking \(I\) symmetry. \(I\) symmetry pins the axion angle \(\theta\) to \(\pi\) even when \(T\) symmetry is broken. AXIs have the quantized magneto-electric effect from the nontrivial axion angle \(\theta = \pi [4–6]\), and the surfaces of AXIs have a half quantum Hall effect [4, 9]. Recently, EuIn2As2 [11] and MnBi2Te4 [14] have been proposed as layered antiferromagnetic TIs, and then they have been studied extensively [15–26]. In MnBi2Te4, the combined symmetry \(S = T_{\tau_1/2}\) leads to a \(Z_2\) topological classification in the absence of \(T\) symmetry [27], where \(T\) and \(\tau_{1/2}\) represent a \(T\) operator and a half-translation one respectively.

Higher-order TIs (HOTIs) have been proposed as a new class of TIs [28–70]. 3D HOTIs have topological one-dimensional states along hinges of the systems, which are called hinge states. Hinge states arise from nontrivial higher-order topology of the bulk. Among various classes of HOTIs, one class of HOTIs is protected by \(I\) symmetry [10, 11, 39, 40, 43–46]. The HOTIs without \(T\) symmetry have chiral hinge states (CHS) [10, 11, 39, 40, 43], whereas the HOTIs with \(T\) symmetry have helical hinge states [44–46, 71]. In the magnetic systems only with \(I\) symmetry, the topological phases are characterized by three weak \(Z_2\) indices and the strong \(Z_4\) index \(\mu_1 [72–77]\), and CHS always appear when all the weak indices vanish and \(\mu_1 = 2 [78, 79]\). Therefore, magnetic TIs with \(I\) symmetry and \(\mu_1 = 2\) have CHS, and remarkably, they are AXIs with \(\theta = \pi [9–11, 13]\). The positions of the CHS found are always \(I\) symmetric [10, 11, 39, 40, 43].

In the present Letter, we found all the possible patterns of positions of CHS in HOTIs from \(I\) symmetry. In particular, we study emergence of \(I\)-asymmetric hinge states (IAHS) in layered antiferromagnetic AXIs. They appear at the \(I\)-asymmetric positions in the case of an even number of layers because \(I\) symmetry is broken. Moreover, we show that IAHS result from the bulk \(Z_4\) topology protected by \(I\) symmetry, and they generally appear in antiferromagnets (AFMs) with an even number of layers and the non-trivial \(Z_4\) index. In addition, we show that their \(I\)-asymmetric positions are uniquely determined from an interplay of the symmetries and topology, which is also discussed in the axion insulator EuIn2As2 [11, 23, 24].

Magnetic space groups with inversion symmetry.—First, we consider positions of the CHS in all the 92 space groups (SGs) with \(I\) symmetry or, equivalently the 92 type-I magnetic space groups (MSGs) with \(I\) symmetry. To this end, we consider a Dirac Hamiltonian on a surface of the system. We first assume that the surface Dirac mass \(m_n\) is determined by the surface orientation, where \(n\) is the normal vector of the surface. We show the dependence of \(m_n\) on \(n\) in a system with a shape of a sphere (Fig. 1). In the \(I\) symmetric HOTIs without \(T\) symmetry, the sign of the mass term is reversed by \(I\) operation, i.e. \(m_n = -m_{-n}\). Thus, the domain wall with \(m_n = 0\) appears in a \(I\)-symmetric manner, and on this \(m_n = 0\) line, CHS appear in a clockwise direction around the region with positive \(m_n\) (see Fig. 1(a-1)). Therefore, in the rod geometry along the \(z\) direction, CHS follows from \(m_n\) on the equator of the sphere (Fig. 1(a-2)).

Next, we consider the cases with \(n\)-fold rotational (\(C_{n_2}\)) symmetry around the \(z\)-axis in addition to \(I\) symmetry. In the presence of \(I\) and \(C_{3z}\) symmetries, i.e. the point group (PG) \(\overline{3}\), the CHS is invariant under \(C_{3z}\) symmetry (Fig. 1(b)). In the cases with \(C_{2z}\) symmetry, the CHS on the sphere is always a great circle on the mirror.
FIG. 1. The distributions of the mass term and CHS on a sphere in all point groups (PGs) with I symmetry. (a-1) The CHS form a loop protected by I symmetry in the PG T, and (a-2) in the rod geometry they appear along the z direction. (b) In the PG 3 the CHS on the sphere are invariant under C_{za} and I symmetries. In PGs (c) 2/m, 4/m, 6/m, (d) mmm, m3, (e) 5m, (f) 4/mmm, (g) 6/mmm, (h) m\bar{3}m, the CHS form one, three, five, seven and nine great circles, respectively.

In this case, chiral surface states protected by mirror symmetry appear on the side surfaces in the rod geometry along the z-axis. Meanwhile, if all the surfaces of the crystal are not mirror symmetric, CHS appear. Furthermore, in the cases with C_{4z} or C_{6z} symmetries, the distributions of the mass terms are the same as those with C_{2z} symmetry. Thus, the CHS on the sphere are along a great circle in the PGs 2/m, 4/m and 6/m. Similarly, in other PGs, the patterns of CHS are classified into the five patterns (Fig. 1(d-h)), where the CHS are located on great circles on the mirror planes.

We identified all the possible patterns for all the 92 type-I MSGs with I symmetry. Using an observation that m_m behaves as a pseudoscalar under PG operations, we can uniquely determine the pattern of mass distribution on a sphere, with its details in the Supplementary Material. Here, we note the following point: so far we assume that the sign of m_m is uniquely determined by the surface orientation, but the assumption is valid only when the system without glide symmetries. For example, we consider a system with a glide symmetry \{M_y|00\frac{1}{2}\}. Suppose the surface mass term m for the (001) surface z = 0 is positive. Then from the glide symmetry, the (001) surface z = 1/2 has a negative mass. Then the glide symmetry requires two terminations for the (001) surfaces to have opposite mass signs, violating our assumption. In this case, we choose one of the two surface terminations to remove this indeterminacy. In the level of the MSGs, it is achieved by discarding the glide symmetry, reducing the original MSG to its subgroup. To summarize, all the possible patterns for the positions of CHS can be exhausted by considering all the SGs with I symmetry, but without such glide symmetries, as discussed in detail in the Supplementary Materials [80]. All the patterns of the CHS for 92 type-I MSGs with I symmetry are shown in Table I.

**Beyond inversion-symmetric hinge states.**—Here, we consider I-symmetric 3D layered antiferromagnetic HOTI with \(\mu_1 = 2\) in the abovementioned case with the PGs T and 3, the positions of the CHS depend on the parity of the number of layers N, and IAHS generally appear in the cases with even N, lacking I symmetry.

Here we consider two crystals with shapes of a parallelepiped with no additional symmetry and of a hexagonal prism with C_{3z} symmetry (Fig. 2(a)). We assume that each layer has I symmetry. First, we consider CHS along the direction of the stacking, i.e. the z direction as shown in Fig. 2(a) which follow from Fig. 1. Here we assume that the number of layers is much larger than the penetration depth of the CHS. In this case, CHS along the stacking direction always emerge irrespective of the number of layers because of the topological property in the bulk, *i.e.* \(\mu_1 = 2\) [78].

Next, we consider behaviors of CHS at the corners A

| PG | Type-I MSG | CHS in Fig. 1 |
|----|------------|---------------|
| T  | 2, 13, 14, 15, 48, 50, 52, 54, 56, 60, 16, 70, 73, 85, 86, 88, 126, 130, 133, 142. | (a-1) |
| 3  | 147, 148, 163, 165, 167, 201, 203, 205, 206, 222, 228, 230. | (b) |
| 2/m | 10, 11, 12, 49, 51, 53, 55, 57, 58, 59, 62, 63, 64, 66, 67, 72, 74, 125, 129, 134, 137, 138, 141, 120, 135, 136, 140. | (c) |
| 4/m | 83, 84, 87, 124, 127, 128, 131, 132, 135, 136, 140. | (d) |
| mmm | 47, 65, 69, 71. | (e) |
| m3 | 200, 202, 204, 222, 226. | (f) |
| 5m | 162, 164, 166, 224, 227. | (g) |
| 4/mmm | 123, 139. | (h) |
| 6/mmm | 191. | (i) |
| m\bar{3}m | 221, 225, 229. | (j) |
FIG. 2. Positions of the CHS and the slab Chern number $C_{\text{slab}}$. (a) The CHS appear along the $z$ direction, i.e. the stacking direction in the rod geometries without and with $C_{3z}$ symmetry. (b) The number of incoming hinge modes should be equal to that of outgoing hinge modes at the corners A and B. There are two possibilities for CHS, (i) and (ii) in both cases with and without $C_{3z}$ symmetry. (c-f) There are four possible patterns of the positions of CHS. The cases with $N = odd$ are in (c) $C_{\text{slab}} = 1$ and (d) $C_{\text{slab}} = -1$. The cases with $N = even$ are in (e) and (f), and IAHS appear in these cases.

and B in Fig. 2(b). At each corner, the number of incoming hinge modes should be equal to that of outgoing hinge modes because otherwise a charge will be accumulated at a corner in proportion with time, due to the fact that each hinge mode provides one-channel conductance. This argument is similar to the one in Ref. [81] applied for chiral edge currents in a two-dimensional (2D) insulating ferromagnet. Therefore, CHS should appear either along (i) or along (ii) between the corners A and B (Fig. 2(b)). In addition, a similar discussion is applicable to the corners C and D. Therefore there are four possible patterns of the positions of CHS as shown in Figs. 2(c-f). In Figs. 2(c) and 2(d), the positions of CHS are $\mathcal{I}$ symmetric.

Cases with an odd number of layers.—First of all, we consider the cases with odd $N$ with the magnetization of each layer given by $\uparrow \cdots \uparrow$, which represents the magnetizations of the individual layers from top to bottom. When $N$ is odd, the system has $\mathcal{I}$ symmetry, and such an $\mathcal{I}$-symmetric 2D slab of a 3D HOTI with $\mathcal{I}$ symmetry is a 2D Chern insulator with the Chern number $C_{\text{slab}} \equiv 1$ (mod 2) from Refs. [10, 39, 79]. In particular, for odd $N$ with $\uparrow \cdots \uparrow \downarrow$ and $\uparrow \cdots \uparrow \downarrow$, we can choose $C_{\text{slab}} = 1$ and $C'_{\text{slab}} = -1$ respectively without losing generality (for details see Supplementary Material), leading to the positions of CHS shown in Figs. 2(c) and 2(d).

Cases with an even number of layers.—Next, when $N$ is even, $\mathcal{I}$ symmetry is broken and $C'_{\text{slab}} \equiv 1$ (mod 2) does not hold. For even $N$ with $\uparrow \uparrow \cdots \uparrow \downarrow \cdots \downarrow$, it can be understood as $\uparrow \cdots \uparrow + \downarrow \cdots \downarrow$, i.e. the composition of odd-$N$ layers with $C'_{\text{slab}} = 1$ and odd-$N$ layers with $C'_{\text{slab}} = -1$. The resulting positions of CHS are shown in Fig. 2(e) because two counter-propagating CHS on the same hinge will hybridize and open a gap. Likewise, for even $N$ with $\uparrow \cdots \uparrow$, the CHS are as shown in Fig. 2(f), which is obtained from Fig. 2(e) via an $\mathcal{I}$ operation. These positions of CHS are not $\mathcal{I}$ symmetric; namely, they are IAHS. Thus, while CHS form a single loop when $N = odd$ (see Figs. 2(c) and 2(d)), IAHS with $C'_{3z}$ symmetry do not form a single loop, but three loops instead (Figs. 2(e) and 2(f)). The difference in the positions of CHS can be observed by transport measurements on the hinges of crystals.

Interestingly, though a slab with even $N$ does not preserve $\mathcal{I}$ symmetry, it has IAHS which are due to bulk topology protected by bulk $\mathcal{I}$ symmetry. It is also interesting that the positions of the IAHS for even $N$ are also uniquely determined in this case, and they are different from those for odd $N$. EuIn$_2$As$_2$ possess a symmetry under the combination of $\mathcal{I}$ and $\mathcal{T} \equiv C_{2z} \mathcal{T}$, from which the Chern number is $C'_{\text{slab}} = 0$ when $N$ is even [82].

Model calculations.—We use a tight-binding model of a layered AFM showing a HOTI phase with $\mu = 2$ in Ref. [40] to study the IAHS. This model is an alternate stacking of layers of the Haldane model within the $xy$ plane with the Chern number $= \pm 1$ [83], and their magnetizations alternate correspondingly. The details of the model and parameters are provided in supplemental materials [84].

We performed calculations of the tight-binding model by using the PythTB package [85]. We show the band structure with $C_{3z}$-symmetric hexagonal rod geometry along the $z$ direction in Fig. 3(a). Its CHS appear at the $C_{3z}$-symmetric positions (see Figs. 3(a-1) and 3(a-2)) in agreement with Fig. 2. Next we calculate the band structure with rod geometry which is finite along the $z$ direction and the $a$ direction (see Figs. 3(b-1) and 3(c-1)), and infinite along the $x$ direction. The results are shown in Figs. 3(b) and 3(c), for $N = odd$ and $N = even$ respectively. When $N = odd$ (Fig. 3(b-2)), the system is $I$ symmetric, and then the positions of CHS are $I$ symmetric in agreement with Fig. 2(c) with $C_{\text{slab}} = 1$. When $N = even$, the system is not $I$ symmetric, and the positions of CHS are as shown in Fig. 3(c-2), that is, IAHS appear with $C_{\text{slab}} = 0$.

The MSG of the tight-binding model is $P6'_3/m'\overline{m'}\overline{c}$ (#194.268). This MSG contains two kinds of symmetry operations: a glide symmetry $\{M_g 00\frac{1}{2}\}$, and a combination of screw and $\mathcal{T}$ operations, $\mathcal{T}\{C_{2z} 00\frac{1}{2}\}$, both of which lead to a sign inversion of the surface Dirac mass on the (001) surface. As we discussed above, if we remove these operations, the MSG becomes $P\overline{3}m1'$ (#164.89) which has a maximum subgroup of SG 147 ($P\overline{3}$), leading to Fig. 1(b) and Fig. 2. Indeed, they perfectly agree with...
FIG. 3. The positions of CHS and the band structures of the tight-binding model. The details of the model and the parameters are provided in the supplemental materials [84]. The real-space distributions of the CHS (a-2) (b-2) and (c-2) are shown as the sizes of the blue dots. (a) Results for hexagonal rod geometry along the z direction. (a-1) Schematic diagram of the layered AFM comprising layers of the Haldane model, and the positions of CHS for hexagonal rod geometry. (a-2) Real-space distribution of zero-energy modes in the \( xy \) plane. (a-3) The band structure. (b-c) Results for rod geometry which is finite along the \( z \) direction. The numbers of the layers are odd in (b) and even in (c). (b-1) and (c-1) are schematic diagrams of CHS. (b-2) and (c-2) are the real-space distribution of zero-energy modes in the red plane in (b-1) and (c-1). When \( N = 41 \) (odd), the positions of CHS are \( \mathcal{I} \) symmetric. When \( N = 42 \) (even), the positions of CHS are not \( \mathcal{I} \) symmetric, that is, IAHS appear. (b-3)(c-3) The band structures.

Further discussions on an axion insulator EuIn\(_2\)As\(_2\)—
According to Ref. [11], EuIn\(_2\)As\(_2\) is a layered antiferromagnetic AXI with the magnetic moment along \( z \) axis (Fig. 4(a-1)). The MSG of EuIn\(_2\)As\(_2\) is \( P6_3/m\overline{m}m'c \) (#194.268), same with our model. Thus, EuIn\(_2\)As\(_2\) is an ideal material to study the emergence of IAHS. Remarkably, the mass term in EuIn\(_2\)As\(_2\) will change its sign under \( \mathcal{I} \), and invariant under \( C_{3z} \), which makes the mass term having an alternate sign between adjacent side surfaces of the hexagonal crystal shown in Fig. 4(a-2) and Fig. 2(c). Moreover, if \( N \) is even which breaks \( \mathcal{I} \) symmetry (Fig. 4(b-1)), CHS will exist in an \( \mathcal{I} \)-asymmetric configuration (Figs. 4(b-2) and 2(e)).

In the AXIs, such as EuIn\(_2\)As\(_2\), a quantized magneto-electric effect is expected. For its observation, we need to attach electrodes so that they are electrically isolated from each other. The CHS can short-circuit them, then obstructing the measurement. Our analysis shows that the case with \( N = \) even may facilitate the measurement since the IAHS consist of multiple loops.

Conclusion.—In summary, we found all the possible configurations of CHS in HOTIs in type-I MSGs with \( \mathcal{I} \) symmetry. The configurations are uniquely determined from each MSG. In particular, we study emergence of IAHS in AXIs realized in layered AFMs with an even number of layers. They appear at the \( \mathcal{I} \)-asymmetric positions because \( \mathcal{I} \) symmetry is broken in the whole system. Nonetheless, IAHS are protected by \( \mathcal{I} \) symmetry in the bulk, and they are characterized by the topological \( Z_4 \) invariant. This difference in positions of CHS can be observed by transport measurements through hinges. Furthermore, we predict that IAHS appear in an AXI EuIn\(_2\)As\(_2\) with an even number of layers.

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[1] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
[2] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
[3] F. Wilczek, Phys. Rev. Lett. 58, 1799 (1987).
[4] X.-L. Qi, T. L. Hughes, and S.-C. Zhang, Phys. Rev. B 78, 195424 (2008).
[5] A. M. Essin, J. E. Moore, and D. Vanderbilt, Phys. Rev. Lett. 102, 146805 (2009).
[6] A. M. Essin, A. M. Turner, J. E. Moore, and D. Vanderbilt, Phys. Rev. B 81, 205104 (2010).
[7] X. Chen, L. Fidkowski, and A. Vishwanath, Phys. Rev. B 89, 165132 (2014).
[8] J. Wang, B. Lian, and S.-C. Zhang, Phys. Rev. B 93, 045115 (2016).
[9] N. Varnava and D. Vanderbilt, Phys. Rev. B 98, 245117 (2018).
[10] B. J. Wieder and B. A. Bernevig, arXiv preprint arXiv:1810.02373 (2018).
[11] Y. Xu, Z. Song, Z. Wang, H. Weng, and X. Dai, Phys.
[63] A. Agarwala, V. Juričić, and B. Roy, Phys. Rev. Research 2, 012067 (2020).
[64] R. Queiroz and A. Stern, Phys. Rev. Lett. 123, 036802 (2019).
[65] R. Chen, C.-Z. Chen, J.-H. Gao, B. Zhou, and D.-H. Xu, Phys. Rev. Lett. 124, 036803 (2020).
[66] T. Fukui and Y. Hatsugai, Phys. Rev. B 98, 035147 (2018).
[67] K. Plekhanov, F. Ronetti, D. Loss, and J. Klinovaja, Phys. Rev. Research 2, 013083 (2020).
[68] A. K. Ghosh, G. C. Paul, and A. Saha, arXiv preprint arXiv:1911.09361 (2019).
[69] M. Hirayama, R. Takahashi, S. Matsuishi, H. Hosono, and S. Murakami, arXiv preprint arXiv:2004.03785 (2020).
[70] C. Chen, J.-Z. Zhao, Z. Chen, Z.-M. Yu, Z. Song, X.-L. Sheng, and S. A. Yang, arXiv preprint arXiv:2004.02787 (2020).
[71] X. Zhou, C.-H. Hsu, C.-Y. Huang, M. Iraola, J. L. Mañes, M. G. Vergniory, H. Lin, and N. Kioussis, arXiv preprint arXiv:2005.06071 (2020).
[72] J. Kruthoff, J. de Boer, J. van Wezel, C. L. Kane, and R.-J. Slager, Phys. Rev. X 7, 041069 (2017).
[73] H. C. Po, A. Vishwanath, and H. Watanabe, Nat. Commun. 8, 50 (2017).
[74] E. Khalaf, H. C. Po, A. Vishwanath, and H. Watanabe, Phys. Rev. X 8, 031070 (2018).
[75] S. Ono and H. Watanabe, Phys. Rev. B 98, 115150 (2018).
[76] F. Tang, H. C. Po, A. Vishwanath, and X. Wan, Nature 566, 486 (2019).
[77] F. Tang, H. C. Po, A. Vishwanath, and X. Wan, Nat. Phys. 15, 470 (2019).
[78] Y. Tanaka, R. Takahashi, and S. Murakami, Phys. Rev. B 101, 115120 (2020).
[79] R. Takahashi, Y. Tanaka, and S. Murakami, Phys. Rev. Research 2, 013300 (2020).
[80] See Supplemental Material at URL for the details of the surface theory of hinge states in 92 SGs with $I$ symmetry.
[81] D. Vanderbilt, *Berry Phases in Electronic Structure Theory: Electric Polarization, Orbital Magnetization and Topological Insulators* (Cambridge University Press, Cambridge, 2018).
[82] See Supplemental Material at URL for the proof that the Chern number is $C^\text{lab}_{\text{slab}} = 0$ when $N$ is even.
[83] F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).
[84] See Supplemental Material at URL for the details of the tight-binding model and parameters.
[85] “Python tight binding open-source package,” http://physics.rutgers.edu/pythtb/.
I. SURFACE THEORY OF CHIRAL HINGE STATES IN 92 TYPE-I MAGNETIC SPACE GROUPS WITH $I$ SYMMETRY

In this appendix, we identified all the possible patterns of the chiral hinge states (CHS) for all the 92 type-I magnetic space groups (MSGs) with $I$ symmetry. We find that in the 59 type-I MSGs out of the 92 type-I MSGs, the CHS appear along great circles on the sphere. The rest of the type-I MSGs is divided into two classes: the class characterized by $I$ symmetry (see Fig. S1(a)) and that characterized by $I$ and $C_{3z}$ symmetries (see Fig. S1(b)).

A. Dirac Hamiltonian on the surfaces of spheres

First, we start from the surface theory of higher-order topological insulators (HOTIs), and from this information, we discuss emergence of CHS. We assume that surfaces of HOTIs with $I$ symmetry, are represented by the Dirac Hamiltonian. In the simplest case, the surface Dirac Hamiltonian $H(k)$ with a mass term is given by

$$H(k_1, k_2) = \lambda(k_1\sigma_2 - k_3\sigma_1) + m\sigma_3,$$

where $\sigma_i$ ($i = 1, 2, 3$) represent the Pauli matrices, $(k_1, k_2)$ is the wave-vector along the surface, and $\lambda$ and $m$ are real constants. Here, $m$ represents the surface Dirac mass. In fact, this form of the Hamiltonian is just an example, and

![FIG. S1. The distributions of the mass term on a sphere and the positions of CHS in the rod geometry.](image-url)

(a) The signs of the mass on the sphere with $I$ symmetry. The mass sign on the equator of the sphere corresponds that on the surface in the rod geometry along the $z$ directions. (b) The case with $I$ symmetry and $C_{3z}$ symmetries. (c) The case with $I$ symmetry and mirror $M_z$ symmetry with respect to $xy$ plane, leading also to $C_{3z}$ symmetry. The chiral edge states flow along the great circle at the intersection between the sphere and the mirror plane. It leads to the surface states in the rod geometry along the $z$ direction. (d) In the case with $M_x$, $M_y$ and $M_z$ symmetries, chiral edge states appear along three great circles, and the surface states appear in the rod geometries along $x$, $y$ and $z$ directions.
FIG. S2. The distributions of the mass term on a sphere in all point groups with $I$ symmetry. The pattern of the gapless line are grouped by the point groups. (a-1) The CHS form a loop protected by $I$ symmetry in the point group $\bar{1}$. (b) In the point group $3$ the CHS on the sphere are invariant under $C_3 \mathbb{Z}$ symmetry and $I$ symmetry. (c) In the point groups $2/m$, $4/m$ and $6/m$, the gapless line is along the great circle protected by mirror $M_\mathbb{Z}$ symmetry. (d) CHS appear along the three great circles because of $M_x$, $M_y$ and $M_z$ symmetries in the point groups $mmm$ and $m\bar{3}$. (e) CHS appear along three great circles which are related by $C_3$ symmetry in the point group $3m$. (f) In the point group $4/mmm$, the gapless line appear along the five great circles because of $M_x$, $M_y$, $M_z$, $M_{xy}$ and $M_{xz}$. (g) In the point group $6/mmm$, seven great circles of gapless lines appear. (h) Nine great circles appear in the point group $m\bar{3}m$. in general cases, the Hamiltonian $\mathcal{H}(k)$ on the surface with a unit normal vector $n$ can be represented by

$$\mathcal{H}(k_1, k_2) = \sum_{i,j=1}^{3} A_{ij} \sigma_i k_j,$$

where $k_3 \equiv m$ is a Dirac mass. In addition, $A_{ij}$ are real, and we can always assume $\det(A) > 0$, because otherwise we change the definition of $m$ by $m \leftrightarrow -m$ so that $\det(A)$ becomes positive. Furthermore, for the moment we assume that the sign of the mass term is determined uniquely by the surface normal vector $n$. Because of $I$ symmetry, the mass term satisfies $m = -m$, that is, the mass term is reversed by $I$ operation. From this, the domain wall with $m = 0$ appear between the regions with a positive $m$ and that with a negative $m$ (see Figs. S1(a) and S1(b)). Along this massless line, CHS exist in a clockwise way around the $m > 0$ region.

The distributions of $m$ on a sphere include the informations of the positions of CHS in the rod geometry. As shown in Fig. S1(a), $m$ on the surfaces of the rod geometry along the $z$ direction, is determined by the distribution of $m$ on the equator of the sphere. Next, we consider the case with $I$ and $C_{3\mathbb{Z}}$ symmetries. It leads to the positions of CHS shown in Fig. S1(b). We consider the case with $I$ symmetry and mirror $M_\mathbb{Z}$ symmetry with respect to $xy$ plane, leading to the concomitant $C_{2\mathbb{Z}}$ symmetry. In this case, the chiral edge mode is along a great circle on the sphere along the mirror plane as shown in Fig. S1(c) because the sign of the mass flips under improper rotation, such as mirror operation. It leads to the surface states in the rod geometry along the $z$ direction. These gapless surface states are protected by mirror symmetry. Meanwhile if all the surfaces of the crystal is not mirror symmetric, CHS appear. In the case with $M_x$, $M_y$ and $M_z$ symmetries, the surface states appear in the rod geometries along $x$, $y$ and $z$ directions (Fig. S1(d)). In this way, the mass term on a sphere includes various informations of positions of CHS, and then in the following we consider the distributions of mass term on spheres with various symmetries.

B. Various cases of the distribution of the mass term classified by symmetries

1. Rotation and screw rotation symmetries

As discussed above, the CHS form a loop protected by $I$ symmetry in the point group $\bar{1}$ without other symmetries (Fig. S2(a-1)). Here, we add rotation $C_{n\mathbb{Z}}$ ($n = 2, 3, 4, 6$) symmetries around $z$ axis. The mass signs do not flip under rotations. In the case with $C_{3\mathbb{Z}}$ symmetry, that is, in point group $3$, the CHS on the sphere are invariant under...
TABLE S1. The patterns of the CHS on the sphere for 92 type-I MSGs with $I$ symmetry, are grouped into eight configurations shown in Fig. S2. The CHS form loops which are not great circles only in point groups $I$ and $3$. In other point groups, the CHS form great circles. The type-I MSG numbers with an underline indicate the MSG without glide symmetry. For the type-I MSGs containing glide symmetry, we need to remove all the glide symmetry from the type-I MSGs, and we classify them by the point group with which the resulting subgroup is associated.

| Point group name | Point group symbol | Type-I MSG numbers | CHS in Fig. S2 |
|------------------|--------------------|--------------------|---------------|
| $I$              | $C_i$              | $2, 13, 14, 15, 48, 50, 52, 54, 56, 60, 61, 68, 70, 73, 75, 86, 88, 126, 130, 133, 142$. | (a-1) |
| $3$              | $S_6$              | 147, 148, 163, 165, 167, 201, 203, 205, 206, 222, 228, 230. | (b) |
| $2/m$            | $C_{2h}$           | 10, 11, 12, 49, 51, 53, 55, 57, 58, 59, 62, 63, 64, 66, 67, 72, 74, 125, 129, 134, 137, 138, 141. | (c) |
| $4/m$            | $C_{4h}$           | 83, 84, 87, 124, 127, 128, 131, 132, 135, 136, 140. | |
| $6/m$            | $C_{6h}$           | 175, 176, 192, 193, 194. | (d) |
| $mmm$            | $D_{2h}$           | 47, 65, 69, 71. | |
| $m\bar{3}$      | $T_h$              | 200, 202, 204, 223, 226. | (e) |
| $3m$             | $D_{3d}$           | 162, 164, 166, 224, 227. | |
| $4/m\overline{mmm}$ | $D_{4h}$      | 123, 139. | (f) |
| $6/m\overline{mmm}$ | $D_{6h}$      | 191. | (g) |
| $m\bar{3}m$     | $O_h$              | 221, 225, 229. | (h) |

$C_{3z}$ symmetry and $I$ symmetry as shown in Fig. S2(b). On the other hand, in the case with $C_{2z}$ symmetry, the combination of $I$ symmetry and $C_{2z}$ symmetry leads to the mirror $M_z$ symmetry with respect to $xy$ plane, and the gapless line is along the great circle on the mirror plane (Fig. S2(c)). The same applies to the case with $C_{4z}$ and $C_{6z}$ symmetries.

Next we consider screw symmetries. we are assuming that mass distributions are determined only by the normal vectors on the sphere. Therefore, the mass distributions are not affected by the fractional translation operation, and therefore the mass distributions in the presence of screw rotation symmetries are the same as that with the corresponding rotation symmetries by omitting the fractional translations. In summary, the pattern of the chiral edge states for type-I MSGs with proper rotations only are grouped by the point groups, and the chiral edge states on the sphere are along a great circle in the point groups $2/m$, $4/m$ and $6/m$.

2. Mirror and glide symmetries

Here we consider cases with mirror and glide symmetries. The sign of the mass on the sphere flips under improper rotations such as mirror and glide operations, since an $I$ operation flips the sign of the mass. Here, unlike proper rotations, we should treat mirror and glide operations differently. The mirror reflections have been treated in the previous subsection, and the chiral edge states appears on a great sphere on the mirror plane, because on the great circle the mass vanishes. On the other hand, existence of glide operation invalidates our assumption that the surface orientation specified by $n$ uniquely determines the sign of the mass. For example, let us consider the glide $G = \{M_y|[00\frac{1}{2}]\}$. Then, if the mass on the $z = 0$ surface is positive, the mass on the $z = 1/2$ surface is negative. Thus, the mass sign depends on a choice of surface terminations. In this case, in order to proceed, we choose one of the surface terminations. This fixing of surface termination corresponds to removing the glide symmetry from the MSG considered.

Type-I MSGs have various kinds of glide symmetries, and one can see that in every glide symmetry there is one surface orientation $n$ which has both positive and negative mass signs depending on surface terminations. Thus,
to summarize, we need to remove all the glide symmetries from the MSGs, and consider the remaining symmetry operations to determine the positions of CHS. Then, the mass distribution are classified by the point groups in the absence of glide symmetry. In the point groups $mmm$ and $m\overline{3}$, CHS appear along the three great circles because of $M_x$, $M_y$, and $M_z$ symmetries with respect to $x$, $y$, and $z$ axes respectively (see Fig. S2(d)). In addition, CHS appear along three great circles which are related by $C_{4z}$ symmetry in the point group $3m$ as shown in Fig. S2(e). The point group $4/mmm$ has two mirror symmetries $M_{xy}$ and $M_{yz}$ that leave the $x = -y$ and the $x = y$ planes invariant respectively in addition to the mirror symmetries $M_x$, $M_y$, and $M_z$. Because of these mirror symmetries, CHS appear along the five great circles as shown in Fig. S2(g). In the point groups $6/mmm$ and $m\overline{3}m$, seven and nine great circles of gapless lines appear respectively because of additional mirror and rotation symmetries (Figs. S2(g) and S2(h)).

In summary, the patterns of CHS on the sphere for 92 type-I MSGs are grouped in terms of the corresponding point groups. For the MSGs containing glide symmetries, we need to remove all the glide symmetries from the MSGs, and then classify them by their point groups with which the resulting subgroup is associated. All the patterns of the CHS for 92 type-I MSGs with $I$ symmetry are shown in Table S1. In the 59 type-I MSGs, the CHS are along great circles, in the rest of the type-I MSGs with $I$ symmetry, the CHS form a loop which is not a great circle. In these 33 type-I MSGs, the loops of CHS are classified into two patterns characterized by point groups $I$ and $\overline{3}$.

II. PROOF OF $C_{\text{slab}}^z = 0$ WHEN $N$ IS AN EVEN NUMBER

We define a 2D Chern number $C_{\text{slab}}^z$ as

$$C_{\text{slab}}^z = \frac{1}{2\pi} \int_{BZ} dk_x dk_y \text{Tr} [F_{xy}(k)]. \quad (S3)$$

Here

$$F_{ab}(k) = \partial_a A(k) - \partial_b A(k) - i [A_a(k), A_b(k)] \quad (S4)$$

is the non-Abelian Berry curvature written in terms of the Berry connection of the occupied bands for the $\alpha$ type layers, $(A_\alpha(k))_{nm} = i \langle u_n(k) | \partial_\mu | u_m(k) \rangle$.

Here, we show that a Chern number is $C_{\text{slab}}^z = 0$ for a slab of layered antiferromagnets (AFMs) with the even number of layers. In the following, $N$ represents a number of the layers. In the following, we show the relation $C_{\text{slab}}^z = -C_{\text{slab}}^z$ via the combination of $I$ and an anti-unitary operation $\overline{T} = C_{2z}T$, where $T$ represents a time-reversal operation and $C_{2z}$ represents a two-fold rotation around $z$-axis as shown in Fig. S3. Slabs with even $N$ are symmetric under the combination of a unitary operation $I$ and an anti-unitary operation $\overline{T}$:

$$\overline{T}I\mathcal{H}(k)(\overline{T}I)^{-1} = \mathcal{H}(-k), \quad (S5)$$

where $\mathcal{H}(k)$ is the Hamiltonian of the slab with even $N$. From this, for an occupied state $|u_n(k)\rangle$ of the Hamiltonian $\mathcal{H}(k)$ with an eigenvalues $E_n$, the following relation holds:

$$\mathcal{H}(-k)\overline{T} |u_n(k)\rangle = \overline{T}I\mathcal{H}(k) |u_n(k)\rangle = E_n \overline{T}I |u_n(k)\rangle. \quad (S6)$$

![FIG. S3. Two symmetry operations on a slab of a layered AFM with an even number of layers. The slab with even $N$ and its inversion partner connected by the inversion operation $I$. The Chern number of the two slabs are the same. In addition, the slab with even $N$ and its inversion partner connected by the anti-unitary operation $\overline{T}$. The Chern number of the two slabs are of the opposite signs.](attachment:FIG_S3.png)
Therefore, \( \tilde{T} |u_n(k)\rangle \) is an eigenstate of the Hamiltonian \( \mathcal{H}(-k) \), and we can expand
\[
\tilde{T} |u_n(k)\rangle = \sum_m U_{mn}(k) |u_m(-k)\rangle ,
\]
where \( U_{mn}(k) \) are the matrix elements of a unitary transformation acting on the space of occupied states. Because of the anti-unitarity of \( \tilde{T} \), we obtain
\[
|u_n(k)\rangle = \sum_m U^*_{mn}(k) |\tilde{T} u_m(-k)\rangle .
\]
Therefore, the Berry connection is expressed as
\[
(A_{\mu}(k))_{nn'} = i \sum_m U_{mn}(k) \langle \tilde{T} u_m(-k) | \partial_{\mu} \left( \sum_{m'} U^*_{m'n'}(k) |\tilde{T} u_{m'}(-k)\rangle \right)
= - \sum_{m,m'} U^*_n m'(k) (A_{\mu}(-k))_{m'm} U_{mn}(k) - i \sum_m U^*_n m'(k) \partial_{\mu} U_{mn}(k)
= -(U^1(k)(A_{\mu}(-k))U(k))_{nn'}^T - i(U^1(k)\partial_{\mu} U(k))_{nn'}^T ,
\]
and then the Berry curvature is written by
\[
\mathcal{F}_{ab}(k) = -(U^1(k)\mathcal{F}_{ab}(-k)U(k))^T .
\]

Therefore, we obtain the relationship \( C_{\text{slab}}^z = -C_{\text{slab}}^y \). We note that this proof is based on the existence of the anti-unitary operation \( \tilde{T} \), which interchanges the slab with even \( N \) and its inversion partner (see Fig. S3). In other layered AFMs with an anti-unitary operator \( \tilde{T} \) such as \( \tilde{T} = C_{3z} T, C_{4z} T \) or \( C_{6z} T \), the Chern number of the even slab is zero.

### III. Chern Number for a 2D Slab from a 3D HOTI

According to the previous works\(^{1-4}\), a two-dimensional (2D) slab of a 3D HOTI with inversion symmetry, with a finite thickness along the \( z \) direction is a 2D Chern insulator with the Chern number \( C_{\text{slab}}^z = 1 \) (mod 2). In particular, in the case of the layered insulating AFM, when \( N = \text{odd} \), \( \mathcal{I} \) symmetry is preserved, and the slab Chern number \( C_{\text{slab}}^z \) (mod 2) satisfies\(^3\);
\[
C_{\text{slab}}^z = \frac{1}{2} \mu_1 \text{ (mod 2)} ,
\]
where \( \mu_1 = 0 \) or \( 2 \) (mod 4). Therefore, when \( \mu_1 = 2 \) in the bulk, the slab system with odd \( N \) is a 2D Chern insulator with \( C_{\text{slab}}^z = 1 \) (mod 2), i.e. \( C_{\text{slab}}^z = 2M + 1 \).

Nonetheless, we can choose \( C_{\text{slab}}^z = 1 \) without losing generality. One can simultaneously attach two 2D Chern insulators with the same Chern number on two surfaces of the opposite sides of the crystal, so that \( \mathcal{I} \) symmetry is preserved. This procedure is similar to that in Refs.\(^{1,2,5}\). From this, a Chern number = \( 2M + 1 \) can be transformed into a Chern number = 1 while preserving \( \mathcal{I} \) symmetry. Thus, in the main text, we choose the \( C_{\text{slab}}^z = 1 \).

In addition, we consider Chern numbers in the slabs with a finite system size along the \( x \) and \( y \) directions; \( C_{\text{slab}}^x \) and \( C_{\text{slab}}^y \). Here we assume the crystal shapes are \( \mathcal{I} \) symmetric. In this case, we obtain the Chern numbers \( C_{\text{slab}}^x \) and \( C_{\text{slab}}^y \) form the topological \( Z_4 \) index \( \mu_1 \) as
\[
C_{\text{slab}}^z = \frac{1}{2} \mu_1 \text{ (mod 2)},
\]
where \( \mu_1 \) is even\(^{2,3}\). Therefore, the HOTI with \( \mu_1 = 2 \) is a 2D Chern insulator in the case with a finite thickness along the \( x \) and \( y \) directions. Indeed, as shown in Fig. S4(a) and S4(b), the projections of CHS onto the \( yz \) or \( xz \) planes form loops corresponding to the Chern numbers \( C_{\text{slab}}^x \equiv C_{\text{slab}}^y \equiv 1 \) (mod 2), in both cases with odd and even \( N \). Therefore, IAHS (for even \( N \)) are topological gapless states characterized by
\[
C_{\text{slab}}^z \equiv C_{\text{slab}}^y \equiv C_{\text{slab}}^z \equiv 1 \text{ and } C_{\text{slab}}^x \equiv 0 \text{ (mod 2)} .
\]

This topological properties of IAHS are different from that of conventional \( \mathcal{I} \)-symmetric hinge states for odd \( N \), i.e. \( C_{\text{slab}}^x \equiv C_{\text{slab}}^y \equiv C_{\text{slab}}^z \equiv 1 \). We note that the relationship \( C_{\text{slab}}^x \equiv C_{\text{slab}}^y \equiv C_{\text{slab}}^z \equiv 1 \) (mod 2) is due to the bulk topology \( \mu_1 = 2 \), and the 2D Chern numbers remain nontrivial as long as the topological invariant \( \mu_1 \) in the bulk is preserved.
IV. 3D TIGHT-BINDING MODEL

We use a tight-binding model of a layered AFM showing a HOTI phase to study the behaviors of the IAHS. This model was proposed as a model with CHS in Ref. 6. This model is constructed by stacking layers of the Haldane model7 as shown in Figs. S5(a) and S5(b). The Haldane model is a tight-binding model on the honeycomb lattice representing a ferromagnet, and its Hamiltonian within the α-th layers is written as

\[ H_{xy} = t_1 \sum_{\langle ij \rangle, \alpha} c_{i\alpha}^\dagger c_{j\alpha} + i t_2 \sum_{\langle\langle ij \rangle\rangle, \alpha} (-1)^\alpha \nu_{ij} c_{i\alpha}^\dagger c_{j\alpha}, \]  

(S14)

where \( i \) and \( j \) run over the sites in the layer \( \alpha \), \( t_1 \) is the hopping strength for the first-neighbor pairs \( \langle ij \rangle \), \( t_2 \) is that for the second-neighbor pairs, and \( \nu_{ij} = 1 \) ( \( \nu_{ij} = -1 \) ) if the second-neighbor hopping path is counterclockwise (clockwise) in the hexagonal plaquette. The Fermi energy is set to be \( E_F = 0 \). We assume \( t_1 \) and \( t_2 \) to be negative; then this system is a Chern insulator with the Chern number \( C = (-1)^{\alpha+1} \). Therefore, the Chern numbers of the individual layers changes alternately, and so does their magnetization. Therefore, the model is a layered AFM. Next

![FIG. S5. Tight-binding model of the layered AFM.](image)
FIG. S6. The positions of CHS and the band structures of the tight-binding model with parameters \( t_1 = -1 \), \( t_2 = -0.2 \) and \( t_z = -0.3 \). The real-space distributions of the CHS in (a-2) (b-2) and (c-2) are shown as the size of the blue dots. (a) Results for rod geometry along the \( z \) direction. (a-1) schematic diagram of CHS. (a-2) real-space distribution of zero-energy modes in the \( xy \) plane. The longest diagonal length of the hexagonal system in the real space is \( L_1 = 25a \). (a-3) The band structure. (b,c) Results for rod geometry which is finite along the \( z \) and \( a_2 \) directions, and infinite along the \( a_1 \) direction. The lengths of the system along the \( a_2 \) are \( L_2 = 25a \) in both (b) and (c), and those along the \( a_3 \) are \( L_3 = 40a \) (\( N = 41 \)) in (b) and \( L_3 = 41a \) (\( N = 42 \)) in (c). The numbers of the layers are odd in (b) and even in (c). (b-1) and (c-1) are schematic diagrams of CHS. (b-2) and (c-2) are the real-space distribution of zero-energy modes in the red plane in (b-1) and (c-1). (b-3) and (c-3) The band structures. When \( N = \text{odd} \), the positions of CHS are \( I \) symmetric. When \( N = \text{even} \), the positions of CHS i.e. IAHS are not \( I \) symmetric. These model calculations were performed using the PythTB package\(^1\). We introduce a hopping \( t_z \) between the layers as shown in Fig. S5(b), and this Hamiltonian is given by

\[
H_z = \frac{t_z}{2} \sum_{i \in A, \alpha} (1 - (-1)^\alpha)c_{i \alpha}^\dagger c_{i+1 \alpha} + \frac{t_z}{2} \sum_{i \in B, \alpha} (1 + (-1)^\alpha)c_{i \alpha}^\dagger c_{i+1 \alpha} + \text{h.c.} \tag{S15}
\]

The overall Hamiltonian is \( H = H_{xy} + H_z \), and it has \( I \) symmetry in the bulk. This interlayer coupling breaks \( S \) symmetry but preserves bulk inversion symmetry, which leads to gapped surface states and CHS. Here, we assume that the interlayer coupling is weak so that the gap remains open even when \( t_z \) is continuously changed to zero. Then the topological properties of the layered system are the same as those of a stack of decoupled 2D Chern insulators. Therefore, \( C_{\text{slab}} \) is obtained by the sum of the Chern number of each layer.

In 3D systems, there are eight time-reversal invariant momenta (TRIM) denoted by \( \Gamma_j \). The topological phases are characterized by the \( \mathbb{Z}_4 \) index for \( I \) symmetric systems in class A, one of Altland-Zirnbauer symmetry classes\(^8\). The \( \mathbb{Z}_4 \) index is defined as\(^9\)

\[
\mu_1 \equiv \frac{1}{2} \sum_{\Gamma_j: \text{TRIM}} [n_+(\Gamma_j) - n_-(\Gamma_j)] \pmod{4}, \tag{S16}
\]

where \( n_{\pm}(\Gamma_j) \) is the number of the occupied states with even- and odd-parity eigenvalues at the TRIM \( \Gamma_j \). The eight TRIM are as shown in Fig. S5(c), and the parity eigenvalues at each TRIM are shown in Fig. S5(d). From these parity eigenvalues, the \( \mathbb{Z}_4 \) topological index is \( \mu_1 = 2 \) in this model, which leads to CHS\(^10\).

In the following, we perform calculations for the tight-binding model using the PythTB package\(^1\). We calculate the band structure with the rod geometry along the \( z \) direction, and the result is shown in Fig. S6(a). This model
has a three-fold rotational ($C_{3z}$) symmetry, and therefore the CHS appear at the positions which are related by $C_{3z}$ symmetry as shown in Figs. S6(a-1) and S6(a-2). Next we calculate the band structure with the rod geometry which is finite along the directions of $z$ axis and of the primitive translation vector $a_2$, and infinite along the $a_1$ direction. The results are shown in Figs. S6(b) and S6(c), for $N = \text{odd}$ and $N = \text{even}$ respectively. When $N = \text{odd}$, the system is $I$ symmetric, and then the positions of CHS are $I$ symmetric as shown in Fig. S6(b-2), and this configuration of CHS arises from $C_{\text{slab}}^z = 1$. When $N = \text{even}$, the system is not $I$ symmetric, and the positions of CHS i.e. IAHS are as shown in Fig. S6(c-2).

1. E. Khalaf, Phys. Rev. B 97, 205136 (2018).
2. A. Matsugatani and H. Watanabe, Phys. Rev. B 98, 205129 (2018).
3. R. Takahashi, Y. Tanaka, and S. Murakami, Phys. Rev. Research 2, 013300 (2020).
4. B. J. Wieder and B. A. Bernevig, arXiv preprint arXiv:1810.02373 (2018).
5. F. Schindler, A. M. Cook, M. G. Vergniory, Z. Wang, S. S. Parkin, B. A. Bernevig, and T. Neupert, Sci. Adv. 4, eaat0346 (2018).
6. S. H. Kooi, G. van Miert, and C. Ortix, Phys. Rev. B 98, 245102 (2018).
7. F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).
8. A. Altland and M. R. Zirnbauer, Phys. Rev. B 55, 1142 (1997).
9. H. C. Po, A. Vishwanath, and H. Watanabe, Nat. Commun. 8, 50 (2017).
10. Y. Tanaka, R. Takahashi, and S. Murakami, Phys. Rev. B 101, 115120 (2020).
11. “Python tight binding open-source package,” http://physics.rutgers.edu/pythtb/.