

Antichiral surface states and Su-Schrieffer-Heeger physics in rutile altermagnets

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We study surface states and domain wall bound states in altermagnets using a rutile-lattice tight-binding model of electrons coupled to a Néel order. We discover that two symmetry-protected Weyl nodal lines in the bulk band structure can give rise to unconventional antichiral surface states—surface states from opposite surfaces propagate in a *parallel* manner, as opposed to the antiparallel manner for the more conventional chiral surface states. We also find that the antichiral surface states can be turned into chiral surface states upon changing the surface termination. The origin of the surface states, the dependence on the surface termination, and key features of domain wall bound states are explained using a map from the altermagnet to a family of a modified Su-Schrieffer-Heeger chain and the associated bulk-boundary correspondence. Our work reveals rutile altermagnets as a promising candidate among very few quantum materials that can support antichiral surface states.

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Introduction. Recently, an emerging class of unconventional collinear antiferromagnets, known as altermagnet, has attracted a lot of attention due to their rich properties and their prospects in spintronic applications [1–3]. $\mathcal{AB}_2$ compounds featuring a three-dimensional (3D) rutile crystal structure have been shown to be a promising platform for altermagnetism. Examples of candidate materials include metallic RuO_2 , insulating MnF_2 , CoF_2 , and ReO_2 [3]. Each unit cell contains two magnetic $\mathcal{A}$ elements residing on two sublattices whose local environments are made distinct from each other by the arrangement of the nonmagnetic $\mathcal{B}$ elements. The magnetic ordering is marked by the onset of a Néel order whose magnetic unit cell coincides with the unit cell of the lattice. Remarkably, the two sublattices are not linked by an inversion operation, but rather linked by a fourfold screw rotation instead; see Fig. 1(a). Consequently, the band structure in the altermagnetic state lacks the Kramers' degeneracy associated with $\mathcal{PT}$ symmetry and exhibits a characteristic d -wave momentum-dependent spin splitting [1–8].

Symmetry plays a crucial role in a diverse range of phenomena in rutile altermagnets. For instance, when the Néel vector points along the [001] crystallographic direction [9,10], the corresponding nonsymmorphic magnetic space group $P4_2/mnm'$ results in multiple Weyl nodal lines (WNL) in the band structure [11–13]. Moreover, the net magnetization and the linear-order anomalous Hall effect are constrained to be zero by the presence of two glide mirror symmetries [11]. The symmetry admits a leading order parameter

which displays the hallmark of a magnetic octupole moment [12,14–16]. Such an octupolar order parameter is closely connected to the rise of a nonlinear magnetoelectric effect starting only at the second order [17] and a nonlinear Hall response beginning only at the third order [18,19]. It can also couple dynamically with the strain field, giving rise to a characteristic signature from a magnon-polaron hybridization [15]. The symmetry can be altered by tuning the Néel vector away from the [001] direction, which activates the linear-order anomalous Hall effect accompanied by a weak ferromagnetism or ferrimagnetism [10,20–24].

The survey of the roles of symmetry brings about the following question: which physical phenomena emerge when the symmetry is reduced by inhomogeneities in the system? In this Letter, we address this question focusing on the electronic spectral properties in the presence of inhomogeneity stemming from interfaces with vacuum and from magnetic domain walls (DW). To study this, we employ a rutile-lattice tight-binding model of electrons coupled to a Néel order on a slab geometry.

We uncover the existence of antichiral surface states (SS): SS on the opposite surfaces of the slab propagate in the *same* direction. This is in contrast with the familiar case of chiral SS, such as the edge states in Chern insulators and the Fermi arc states in Weyl semimetals, which propagate in an antiparallel fashion between two opposite surfaces. Antichiral SS were first theoretically proposed in a variant of the Haldane honeycomb model where the Haldane flux pattern is modified [25]. However, so far, only few quantum materials have been suggested as their potential hosts, including twisted van der Waals multilayers and Dirac systems where the antichiral SS are stabilized by the electron-phonon coupling [26–29]. Our work demonstrates that rutile altermagnets are an alternative quantum-material platform for their realization. In a large-coupling limit, we explain their origin from two WNL in the bulk using a map from the altermagnet to a family of

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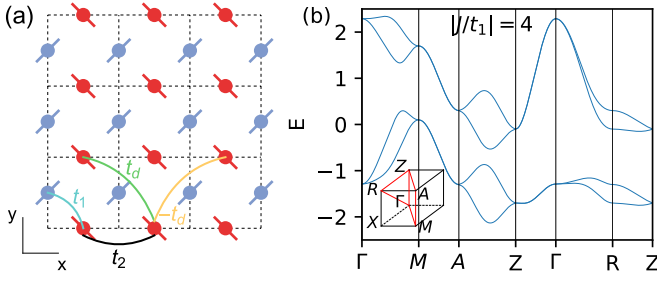


FIG. 1. (a) Illustration of a rutile lattice featuring the two magnetic sublattices, A (blue dots) and B (red dots). They reside on different xy planes and experience different local potentials due to nonmagnetic B sites (not shown), whose impacts are effectively represented by the orientation of the tilted bars. (b) Tight-binding band structure for $\vec{N}_i = \hat{z}$, displaying Weyl nodal lines along MA and ΓZ . [$t_1 = -0.2$, $t_2 = 0.05$, $t'_2 = -0.35$, $t_d = 0.15$ (comparable to the hopping parameters in the single-orbital model for RuO_2 from an *ab initio* study [30]), $J = 0.8$, $\lambda = -0.025$, and $\lambda' = 0.0125$.]

modified Su-Schrieffer-Heeger (SSH) chains. The latter can carry a nontrivial topological invariant, resulting in edge states which are identifiable with the antichiral SS. Using the map, we also explain key features of DW bound states and how the antichiral SS can be switched into chiral SS upon altering the surface termination. We also show how the antichiral SS are stable against an applied Zeeman field and the tilting of the Néel vector into certain directions. Finally, we discuss the possibility of antichiral SS in nonrutile altermagnets.

Model. We consider a 3D electronic tight-binding model for rutile d -wave altermagnets introduced in Refs. [13,30] as a minimal model to study topological properties in the 3D band structure. It is represented by the following Bloch Hamiltonian:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{soc}}, \quad (1)$$

$$\begin{aligned} \mathcal{H}_0 = & -8t_1 c_{x/2} c_{y/2} c_{z/2} \tau_x - 2t'_2 c_z \tau_0 - 2t_2 (c_x + c_y) \tau_0 \\ & - 4t_d s_x s_y \tau_z + J \tau_z \vec{N} \cdot \vec{\sigma}, \end{aligned} \quad (2)$$

$$\begin{aligned} \mathcal{H}_{\text{soc}} = & -8\lambda s_z/2 (s_x/2 c_{y/2} \sigma_x - s_y/2 c_{x/2} \sigma_y) \tau_y \\ & + 16\lambda' c_x/2 c_{y/2} c_{z/2} (c_x - c_y) \tau_y \sigma_z, \end{aligned} \quad (3)$$

where $c_{\alpha/n} \equiv \cos(k_{\alpha}/n)$ and $s_{\alpha/n} \equiv \sin(k_{\alpha}/n)$. The basis vector is $(a_{\vec{k}\uparrow}, a_{\vec{k}\downarrow}, b_{\vec{k}\uparrow}, b_{\vec{k}\downarrow})^T$, where a and b are the annihilation operators on the sublattices A and B [see Fig. 1(a)]. The Pauli matrices, τ_i and σ_i , act on the sublattice and the spin index, respectively. The Néel vector for the i th unit cell is defined by the difference of the magnetic dipole moments on the two sublattices: $\vec{N}_i = \vec{m}_{i,A} - \vec{m}_{i,B}$. $\mathcal{H}_0$ encompasses spin-preserved hoppings and a coupling to a uniform Néel order $\vec{N}_i = \vec{N}$. $\mathcal{H}_{\text{soc}}$ includes hopping due to spin-orbit-coupling effects. Notably, a proper tight-binding description of a rutile altermagnet may require more structures in addition to Eq. (1). For instance, due to a multiorbital character of RuO_2 near the Fermi level, four additional bands must be added to the model in Eq. (1) [30]. However, our formulation can be accordingly generalized to the more complicated cases.

Figure 1(b) shows the band structure for $\vec{N} = \hat{z}$, corresponding to the magnetic point group $4'/mm'm$. It contains a

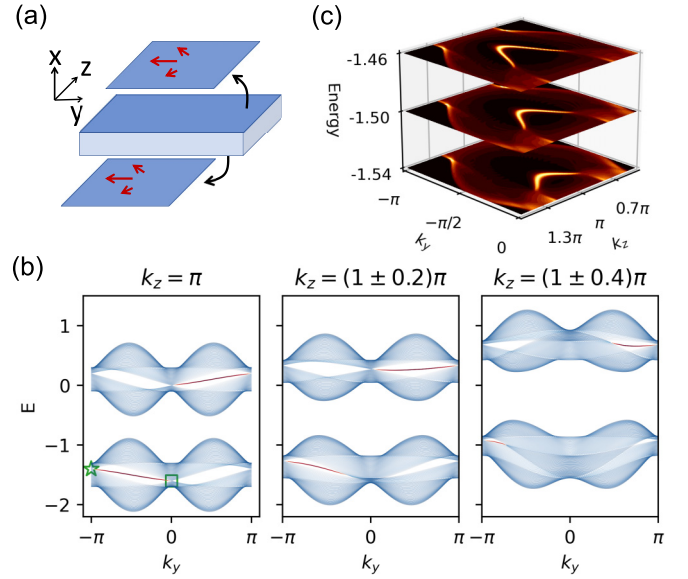


FIG. 2. (a) Schematic illustration of the slab geometry, featuring antichiral SS (red arrows) which propagate predominantly in the negative y direction. (b) Band structures of the slab geometry for $|J/t_1| = 4$, highlighting the in-gap antichiral SS in red. The starting and ending points of the SS curves, e.g., the square and the star, descend from the WNL on ΓZ and MA . (c) Contour plots showing that the antichiral SS, in bright yellow, form open arcs.

twofold rotation z axis and mirror planes $\mathcal{M}_{x,y}$ associated with the nonsymmorphic glide mirrors, $\{\mathcal{M}_x | \frac{1}{2} \frac{1}{2} \frac{1}{2}\}$ and $\{\mathcal{M}_y | \frac{1}{2} \frac{1}{2} \frac{1}{2}\}$. There are Weyl nodes and WNL, whose symmetry protection has been discussed in Refs. [12,13]. In particular, the WNL along ΓZ and MA direction in Fig. 1(b) are protected by the twofold z -axis rotation and the glide mirrors [13]. Next, we show that these WNL can give rise to the antichiral SS in a slab geometry. We emphasize that spin-orbit coupling (SOC) is important for the antichiral SS since the WNL are the results of SOC-induced gapping of preexisting nodal surfaces present in the absence of SOC [31]; for instance, when $\lambda = \lambda' = 0$, the relevant nodal surfaces are in the $k_z k_x$ plane and the $k_y k_z$ plane containing the Γ point as well as the $k_z k_x$ plane and the $k_y k_z$ plane containing the M point.

Antichiral surface states. We consider a slab geometry with open boundaries along the x direction as in Fig. 2(a). The crystal is terminated at A(B) sites for the bottom(top) surface, which is referred to as AB termination. Results for other types and other orientations of the surface termination can be generalized from this. With the remaining two directions of translation invariance, the problem is mapped to one-dimensional (1D) chains parametrized by the crystal momenta k_y and k_z belonging to the surface Brillouin zone, $[-\pi, \pi) \times [-\pi, \pi)$.

Figure 2(b) shows the band structure for a few values of k_z for $\vec{N} = \hat{z}$. The blue continua correspond to the projection of the bulk bands onto the surface Brillouin zone. We observe energy gaps hosting in-gap SS which are exponentially localized to *both* surfaces and represented by the doubly degenerate red curves. In particular, the curve connecting the star and the square in Fig. 2(b) consists of two SS—one for each surface. These SS propagate predominantly

in the same negative y direction, which can be seen from their slope. These are the antichiral SS, as introduced at the beginning. Their unidirectional feature prevails for the whole portion of the parameter space (k_y, k_z) where the SS are observed, as depicted in Fig. 2(c). There, the SS correspond to the bright doubly degenerate open arcs extending from $k_z < \pi$ to $k_z > \pi$. Indeed, they feature the same, predominantly negative group velocity v_y . The red arrows in Fig. 2(a) schematically illustrate the unidirectional behavior. Notably, the antichiral SS propagating in the positive y direction also exist, but they reside at a higher energy, as seen in Fig. 2(b) for $0 < k_y < \pi$. The dependence of the antichiral SS on a few relevant model parameters can be found in the Supplemental Material (SM) [32].

The antichiral SS create a nonzero contribution to the equilibrium charge current, which is necessarily canceled by another contribution from the bulk. As mentioned before, such antichiral SS have been proposed in only a few solid-state systems [26,27,29]. Here, we have clearly demonstrated rutile altermagnets as another natural host. Their physical origin turns out to arise from SSH physics and the associated bulk-boundary correspondence, which is discussed next.

Map to modified SSH chains. The antichiral SS are intimately related to the WNL along ΓZ and MA of the bulk. For instance, the starting and the ending point of the surface-state curve in Fig. 2(b), i.e., the square and the star, descend from the nodal lines upon their projection onto the surface Brillouin zone. We will derive a map from our altermagnetic system to a family of modified SSH chains, which sheds light on the roles of the nodal lines and the rise of the antichiral SS.

To see the map, we proceed in two steps. First, the map is most transparent in the large J limit, where the full band structure decouples into two two-band sectors—one at a lower energy and one at a higher energy. The leading term in the Hamiltonian is the coupling to the Néel vector $\vec{N} = \hat{z}$, and the rest may be viewed as perturbations. From this, we derive effective Hamiltonians for the low-energy and the high-energy sector. Without loss of generality, we focus on the low-energy sector, which is spanned by the -1 eigenvectors of $\tau_z \sigma_z$, namely $\vec{v}_1 = (0, 1, 0, 0)^T$ and $\vec{v}_2 = (0, 0, 1, 0)^T$. In the first order of perturbation, the effective Hamiltonian is

$$\mathcal{H}_L = -2t'_2 c_z - 2t_2(c_x + c_y) - 4t_d s_x s_y \gamma_z - J - 8\lambda s_z/2(s_x/2 c_{y/2} \gamma_y - s_y/2 c_{x/2} \gamma_x), \quad (4)$$

where the Pauli matrices γ_i act on the basis $\{\vec{v}_i\}$.

In the final step, we view k_y and k_z in $\mathcal{H}_L$ as tuning parameters which can be absorbed into the original tight-binding parameters. The outcome is a modified SSH chain [see Fig. 3(a)]:

$$H_{\text{SSH}} = \sum_x (w c_{A,x}^\dagger c_{B,x} + v c_{B,x}^\dagger c_{A,x+1}) + \sum_x [\chi c_{A,x}^\dagger c_{A,x+1} + \chi^* c_{B,x}^\dagger c_{B,x+1}] + \text{H.c.} \quad (5)$$

$w = 4\lambda s_z/2(s_{y/2} + c_{y/2})$, $v = 4\lambda s_z/2(s_{y/2} - c_{y/2})$, and $\chi = -t_2 + i2t_d s_y$. We have ignored terms in $\mathcal{H}_L$ that do not depend on k_x . This is benign for the SS discussion thanks to their topological origin. We have also performed a gauge transformation, $\mathcal{U}^\dagger \mathcal{H}_L \mathcal{U}$, where $\mathcal{U} = e^{-ik_x/4}(\cos \frac{k_x}{4} \gamma_0 + i \sin \frac{k_x}{4} \gamma_z)$. In

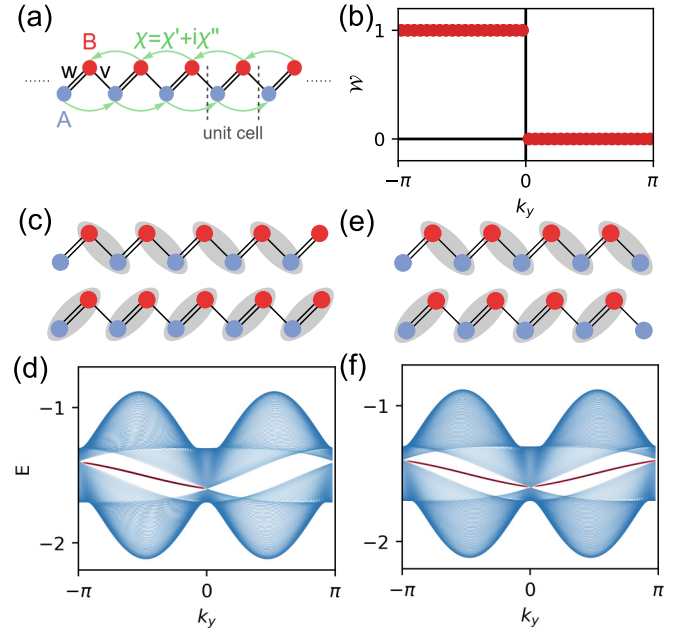


FIG. 3. (a) Real-space representation of the modified SSH chain. (b) k_y dependence of the Z_2 topological invariant $\mathcal{W}$ for the valence band of $\mathcal{H}_{\text{SSH}}$. Panels (c) and (e) illustrate the dimerized limits for the AB and the AA surface termination, respectively. Unpaired outermost sites are identifiable with the SS. Panels (d) and (f) are the band structures of the low-energy sector for the AB and the AA termination, respectively, for $k_z = \pi$. We observe a change from antichiral to chiral SS between the two types of surface termination.

reciprocal space,

$$\mathcal{H}_{\text{SSH}} = \begin{pmatrix} \chi e^{ik_x} + \chi^* e^{-ik_x} & w + v e^{ik_x} \\ w + v e^{-ik_x} & \chi e^{-ik_x} + \chi^* e^{ik_x} \end{pmatrix}. \quad (6)$$

The nonzero χ differentiates our model from the original SSH chain [33]. The SSH chain is known to be a bulk obstructed atomic insulator, which is topologically trivial in the sense that it is smoothly connected to an atomic limit [34–38]. Nevertheless, it supports nontrivial SS arising from a nontrivial bulk topological invariant, in accordance with a bulk-boundary correspondence [39]. Defining such a topological invariant generally requires some care, as addressed in Ref. [39]. The relevant topological invariant for our consideration is the following bulk Z_2 index:

$$\mathcal{W} = \gamma/\pi \bmod 2. \quad (7)$$

$\gamma = i \oint dk_x \langle \alpha(k_x; k_y, k_z) | \partial_{k_x} | \alpha(k_x; k_y, k_z) \rangle$, where $|\alpha\rangle$ is the eigenstate for the valence band of $\mathcal{H}_{\text{SSH}}$ Eq. (6), assumed to be smooth and periodic, $|\alpha(k_x)\rangle = |\alpha(k_x + 2\pi)\rangle$. γ is the so-called intercellular part of the original Zak phase that enters the bulk-boundary correspondence [39,40].

Figure 3(b) shows the k_y dependence of $\mathcal{W}$, which jumps at $k_y = 0$ and π due to the bulk gap closing associated with the ΓZ and MA WNL [see Fig. 1(b)]. For $-\pi < k_y < 0$, the nontrivial $\mathcal{W}$ and the bulk-boundary correspondence indeed explain the presence of SS in Fig. 3(d). This provides a clear understanding of the origin of the antichiral SS from the bulk topological invariant. Next, we discuss their dependence on how the surfaces are terminated.

Dependence on surface termination. There are four types of [100] surface termination: AB, AA, BA, and BB. Remarkably, we find that the antichiral SS are supported only in the AB and BA terminations, while they become chiral for the AA and BB terminations; see Figs. 3(d) and 3(f). To understand this feature, we analyze the electronic behaviors in the representative cases of AB and AA terminations. Generalization to the other surface terminations is possible.

The discussion can be made transparent by considering two dimerized limits of Eq. (6): (i) $|v| \gg |w|, |\chi|$ and (ii) $|w| \gg |v|, |\chi|$. Although the dimerized limits may not be reached in general by the altermagnet, they define equivalence classes and serve as abstract reference points which are smoothly deformed into the effective SSH chains in Eq. (6) without closing the energy gap between the two bands. We then use the adiabaticity argument to elucidate the existence of the SS of the altermagnet from the SS in the associated dimerized limits.

The large $|v|$ in (i) leads to a dimerization between the A and B sublattices of neighboring unit cells, defined in Fig. 3(a). Such a process is illustrated in the top row of Fig. 3(c) and is smoothly connected with our case with $\mathcal{W} = 1$. The leftmost A site and the rightmost B site of the AB open chain are left unpaired and hence identifiable with the SS. In contrast, our case with $\mathcal{W} = 0$ is smoothly connected with the dimerized limit (ii), where $|w|$ dominates so that A and B sublattices of the same unit cells form dimers instead. This is illustrated in the bottom row of Fig. 3(c), where the outermost sites participate in dimerization. Therefore, the SS are expected to be absent. The dimerization picture correctly explains the antichiral SS in the AB slab in Fig. 3(d) for $k_z = \pi$, where the window of $-\pi < k_y < 0$ and $0 < k_y < \pi$ correspond to the dimerized limit (i) and (ii), respectively.

We now deploy the dimerization picture for the AA slab, where the outermost sites are A sites; see Fig. 3(e). By viewing the open chains in panel (e) as resulted from removing the rightmost B sites in panel (c), we see that the top(bottom) row in Fig. 3(e) corresponds to the dimerized limit (i) [(ii)]. The SS are derived from the leftmost(rightmost) unpaired A site. This implies that, for the altermagnet and for $k_z = \pi$, the SS are present in both windows: $-\pi < k_y < 0$ and $0 < k_y < \pi$. This is in an excellent agreement with the numerical results in Fig. 3(f). We note that the overall sign of the group velocity of the SS is mainly determined by the energy offset between the gapless points at $k_y = 0$ and π .

The SS of the AA slab are chiral. By altering one outermost layer of the AB slab to obtain the AA slab, we switch from antichiral to chiral SS. Moreover, the contribution from the SS to the equilibrium current has reduced, which subsequently alters the spatial distribution of the equilibrium current in the bulk. The change of the equilibrium current distribution in this context is left for future investigations. We now turn bound states at altermagnetic DWs.

Bound states at altermagnetic domain walls. We consider the AB slab geometry with a Bloch-typed DW of the Néel vector, wherein the Néel vector of the i th unit cell has the form $\vec{N}_i = (0, \sin \theta_i, \cos \theta_i)^T$. For the left domain $i \leq -w_{dw}/2$, $\theta_i = 0$, and for the right domain $i \geq w_{dw}/2$, $\theta_i = \pi$. In the DW region $-w_{dw}/2 < i < w_{dw}/2$, $\theta_i = \pi(2i + w_{dw})/2w_{dw}$. w_{dw} denotes the width of the DW depicted in Fig. 4(a).

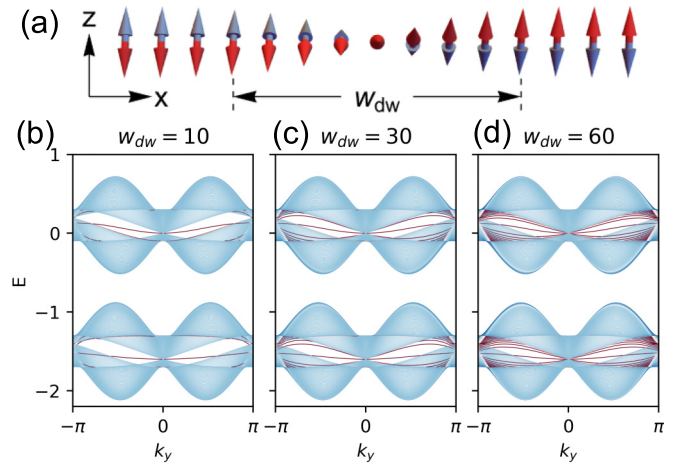


FIG. 4. (a) Illustration of a DW of the Néel vector. Each blue(red) arrow denotes the dipole moment of the A(B) sublattice of a unit cell. (b) Dependence of the band structure at $k_z = \pi$ on the width of the DW, w_{dw} . The DW bound states correspond to the in-gap states (red curves), whose number increases with w_{dw} . When the DW states pass through the continuum bulk states, they hybridize with one another.

Figures 4(b)–4(d) show the band structures for a few values of w_{dw} , featuring (i) continua of bulk states in blue, (ii) in-gap DW bound states in red, and (iii) in-gap SS (omitted). The sharp DW produces mainly one DW bound state within each energy gap, as seen in Fig. 4(b). They have a topological origin, for they can be regarded as the antichiral SS of the left and the right magnetic domains. Upon increasing w_{dw} , more bound states appear, as seen in panels (c) and (d), which is independent of the topological property of the system.

Such behaviors can be understood using a continuum approximation which maps the low-energy sector of the DW problem in the large $|J|$ limit (same for the high-energy sector) into a 1D Dirac fermion model featuring a nonuniform mass (see SM [32] for a derivation):

$$H_{dw} = v_F [i\partial_x \tilde{\gamma}_y + k_y \cos \theta(x) \tilde{\gamma}_x], \quad (8)$$

where $v_F = 4\lambda \sin \frac{k_z}{2}$ and $\tilde{\gamma}_i$'s are Pauli matrices. The mass $v_F k_y \cos \theta(x)$ depends on $\theta(x)$, a continuum version of θ_i . The eigenvalues of H_{dw} describe the energy spectrum close to $k_y = 0$ at a fixed k_z . To gain further insight, we consider a specific DW profile, $\cos \theta(x) = \tanh \beta x$, and employ a Bohr-Sommerfeld quantization condition to obtain the number of DW bound states for the limit $\beta/k_y \rightarrow 0$ (see SM [32] for details):

$$N_b \approx 2 \sqrt{\frac{k_y^2 + |\beta k_y|}{\beta^2}}. \quad (9)$$

Decreasing β in Eq. (9) amounts to increasing w_{dw} , which correctly explains the increasing number of DW bound states while going from panel (b) to (d) in Fig. 4. For a fixed β , the growing N_b with larger $|k_y|$ explains the trend most obvious in Fig. 4(d), where more DW bound states emerge out of the bulk-state continua as one moves away from $k_y = 0$.

Discussion. First, the antichiral SS and their robustness are intertwined with the presence of the symmetry-protected WNL which are stable against an external Zeeman field in

certain high-symmetry directions and the tilting of $\vec{N}$ away from the z axis within certain high-symmetry planes; see the SM [32] and also Ref. [12]. In particular, an external Zeeman field in the x axis or the y axis does not gap out the WNL but rather causes them to move off the high-symmetry paths in the reciprocal space. In such cases, the antichiral SS persist. Otherwise, the WNL are gapped out and the existence of the antichiral SS is no longer guaranteed.

Secondly, as mentioned before, SOC is essential since it gaps out nodal surfaces to produce the WNL. In addition, a larger SOC leads to a more pronounced gap within which the antichiral SS reside. As a result, the antichiral SS become more spatially localized and can be better resolved from the bulk states in the reciprocal space; see Fig. 2 in the SM [32].

Lastly, a group-theory-based study shows that similar WNL exist in a wide range of altermagnets, which includes the rutiles [12]. With such an analogous starting point, antichiral SS could be realized in other altermagnets if situations similar to the rutiles also arise: WNL arrange themselves into pairs. WNL in each pair are parallel to each other so that a slice of the 3D Hamiltonian $\mathcal{H}(\vec{k})$ in the plane perpendicular to the nodal lines can be viewed as an effective 2D Hamiltonian hosting a pair (or pairs) of Dirac cones. The Dirac cones may lead to antichiral SS if there is an energy offset between them. This is the case since each Dirac point corresponds to a topological transition within the SSH framework, as in Fig. 3(b).

Then our results and insights from the rutiles could also be applicable. We leave this prospect for future investigation.

Summary. Our work demonstrates that rutile altermagnets support exotic antichiral SS, which are rare and desirable in quantum materials. Their origin comes from WNL in the bulk bands and is explained using the SSH mapping as well as its bulk-boundary correspondence. In a broader context, our results contribute to the fundamental understanding of altermagnetic systems by establishing a connection between different realms of condensed matter physics. Our work motivates further theoretical and experimental investigation to look for similar antichiral SS in other altermagnetic systems, to examine their robustness against disorder, and to confirm our proposal experimentally, e.g., via angular-resolved photoemission spectroscopy or quasiparticle inference patterns from scanning tunneling microscopy. It also suggests an exciting outlook to explore a potential connection between rutile altermagnets and graphene since the latter is similarly linked to the SSH physics [41].

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