

Electronic structure associated with nonsymmorphic nodal lines in rare-earth tetraborides

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We report a combined microfocused angle-resolved photoemission spectroscopy and first-principles study of the rare-earth tetraborides RB_4 ($R = \text{Tb, Gd}$), which host a Shastry-Sutherland lattice. We identify extended bulk nodal lines at the tetragonal Brillouin-zone boundaries, whose fourfold degeneracies are enforced by the nonsymmorphic glide-mirror symmetries even in the presence of spin-orbit coupling (SOC), unlike conventional nodal lines that SOC typically gaps. Systematically evolving Dirac-like dispersions resolved by momentum-distribution-curve analysis support this symmetry-enforced nodal line. We further identify a related nodal-line feature that disperses toward the Fermi level (E_F); although the calculated SOC-induced gap for this feature (0.2–4.6 meV) lies below the experimental resolution, its proximity to E_F offers a band-structure basis consistent with the emergence of large magnetoresistance. First-principles Wilson-loop calculations establish a nontrivial π Berry phase for the bulk nodal line, and we observe a photon-energy-independent surface-derived feature whose dispersion is consistent with the calculated surface state. Our results identify RB_4 as a platform for nonsymmorphic-symmetry-enforced nodal-line physics with potential relevance to large magnetoresistance and topological surface states.

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I. INTRODUCTION

Topological nodal-line semimetals (TNLSMs) represent a unique class of materials where the conduction and valence bands cross along continuous lines in momentum (k) space [1–9]. Unlike the pointlike crossings found in Weyl or Dirac semimetals, these line crossings induce distinctive physical phenomena, including giant magnetoresistance [10–14], highly field-dependent zero-energy Landau levels [15,16], flat optical conductivity [17,18], and high chemical catalysis performance [19,20]. Furthermore, the bulk-boundary correspondence in TNLSMs gives rise to “drumhead” surface states (SS), flat bands localized on the surface that create a massive density of states (DOS) [1,3,5,21]. This surface-localized DOS enhancement is theoretically predicted to serve as a

fertile platform for exotic phases such as surface superconductivity and charge-density waves [22–25].

While numerous TNLSMs have been identified to date, the majority rely on the “accidental” band crossing protected by point-group symmetries [3–7,9,21,26–41]. In such accidental TNLSMs, the energy of the nodal line relative to the Fermi level (E_F) is highly sensitive to external parameters, such as chemical composition and lattice constants, necessitating delicate fine-tuning to explore the underlying nodal physics. Furthermore, these accidental crossings are inherently fragile; for instance, spin-orbit coupling (SOC) often lifts the degeneracy and opens a gap, thereby hindering the realization of truly gapless topological states [4,5,29–31,37,42–44]. Recent angle-resolved photoemission spectroscopy (ARPES) studies have demonstrated that nonsymmorphic symmetry can stabilize nodal-line features that are robust against SOC and located near E_F , as exemplified by LaSbTe [45]. However, these systems are nonmagnetic and thus do not address how such symmetry-protected nodal lines evolve in the presence of magnetic order. Consequently, magnetic materials hosting nonsymmorphic nodal-line electronic structures near E_F provide an attractive platform for exploring the coexistence of crystalline-symmetry-enforced band degeneracies and magnetic order.

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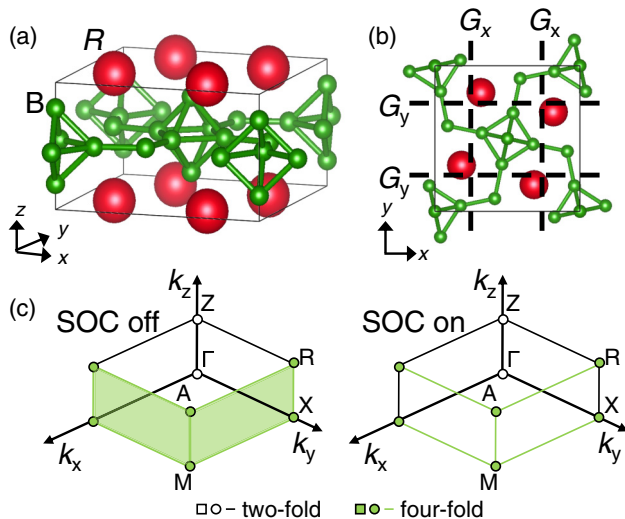


FIG. 1. (a) Crystal structure of RB_4 (R : rare earth). (b) Top view of the crystal structure highlighting the (001) plane. Glide-mirror planes are indicated by black dashed lines. (c) Tetragonal bulk BZ of RB_4 . The k regions where the energy bands show fourfold degeneracy are highlighted by green shades and green lines for without-SOC and with-SOC cases, respectively.

The geometry of nodal trajectories presents another critical frontier. While representative TNLSMs typically host closed nodal loops, certain nonsymmorphic symmetries enforce “open” nodal lines that traverse the entire Brillouin zone (BZ) [46–48]. These nonsymmorphic-enforced degeneracies are theoretically predicted to exhibit exceptional resilience against SOC [49]. However, establishing the bulk-boundary correspondence for such open trajectories remains nontrivial, as the absence of a closed manifold [1,3,5,21] complicates the identification of topological invariants and their associated surface states [50,51]. Experimental evidence for the topological nature of open nodal lines remains less definitive than for their closed-loop counterparts.

In this article, we demonstrate that the rare-earth tetraborides RB_4 ($R = \text{Tb, Gd}$), which undergo antiferromagnetic (AFM) transition at 42–44 K [52–54], serve as an ideal platform to address these challenges. As shown in Figs. 1(a) and 1(b), RB_4 crystallizes in a Shastry-Sutherland lattice [55] with a space group 127 ($P4/mbm$) [Fig. 1(a)], where two orthogonal glide-mirror symmetries, $G_x = \{M_x | 0\frac{1}{2}0\}$ and $G_y = \{M_y | \frac{1}{2}00\}$, play a pivotal role. Our symmetry analysis reveals that these nonsymmorphic glides enforce fourfold band degeneracies along the BZ boundaries [Fig. 1(c)]. By combining microfocused ARPES with first-principles calculations, we experimentally show that these nodal lines exhibit significant energy dispersion that naturally crosses E_F . This intrinsic alignment provides a band-structure basis consistent with the extreme magnetoresistance (MR) reaching $\sim 10^5\%$ reported for this family. Berry-phase calculations further establish the nontrivial topology of these open nodal trajectories, and a photon-energy-independent surface-derived feature we observe is consistent with the associated calculated surface state.

II. EXPERIMENTS AND CALCULATIONS

High-quality single crystals of RB_4 ($R = \text{Tb, Gd}$) were grown by the floating zone or the flux method with Al flux. The details were described elsewhere [56]. Vacuum-ultraviolet ARPES measurements were performed using a Scienta-Omicron DA30 spectrometer at BL-28A in Photon Factory (PF), KEK, with a microfocused beam spot of $10 \times 12 \mu\text{m}^2$ [57]. Circularly polarized photons with photon energies of $h\nu = 100\text{--}150$ eV were used to systematically map the band structure in the three-dimensional BZ. Energy and angular resolutions were set to be 20–30 meV and 0.2° , respectively. Soft x-ray (SX) ARPES measurements were conducted with a Scienta-Omicron SES2002 electron analyzer with energy-tunable synchrotron light at BL-2A in KEK-PF. We used linearly polarized light (horizontal polarization) of 280–580 eV, with an energy resolution of around 150 meV. ARPES measurements were conducted in the paramagnetic (PM) phase ($T = 50$ K), and data near the Fermi level (E_F) were also measured in the AFM phase ($T = 7$ K). Samples were cleaved *in situ* along the (001) plane and measured under an ultrahigh vacuum better than 1×10^{-10} Torr. The crystal orientation was determined by x-ray backscattering measurement, which confirmed the apparent fourfold rotational symmetry of the samples, consistent with the (001) cleaved plane. First-principles band-structure calculations were conducted using QUANTUM ESPRESSO code within the generalized gradient approximation scheme using PSLibrary [58–62]. The experimental lattice parameters and the Wyckoff positions determined by x-ray diffraction and x-ray absorption fine structure measurements, respectively, were used [63,64]. The spin-orbit coupling was included consistently in calculating electronic structures, and a uniform k -point mesh $8 \times 8 \times 12$ was employed for Wannierization. In the Berry-phase calculations for the degenerate bands, the wavefunctions for cuts 1 ($k_y = 0$) and 11 ($k_y = \pi$) in Fig. 3 can be classified according to the glide symmetry. We therefore decomposed the degenerate bands into the corresponding glide-symmetry sectors and evaluated the Berry phase in each sector.

III. FERMI SURFACE AND BAND DISPERSIONS ALONG HIGH-SYMMETRY LINES

Figure 2(a) shows the ARPES intensity mapping at E_F for GdB_4 as a function of the in-plane wave vectors k_x and k_y , measured in the $k_z = 0$ plane in the PM phase at $T = 50$ K. The corresponding calculated Fermi surfaces (FSs) are displayed in Fig. 2(b). The k_z values were determined from photon-energy-dependent normal-emission soft-x-ray ARPES measurements (see Appendix A for details). The ARPES intensity exhibits a clear fourfold-symmetric distribution, consistent with the symmetry of the bulk tetragonal BZ. The calculations reveal two distinct types of FSs: one centered at the Γ point with a characteristic jigsaw-puzzle-like shape (FS1) and the other centered at the M point consisting of relatively small elongated pockets (FS2). These pockets are assigned as electron pockets. According to the calculated band structure along the Γ -M-X- Γ high-symmetry lines [Fig. 2(d)], FS1 and FS2 in Fig. 2(b) originate from electronlike bands with band minima at the binding energy (E_B) of approximately

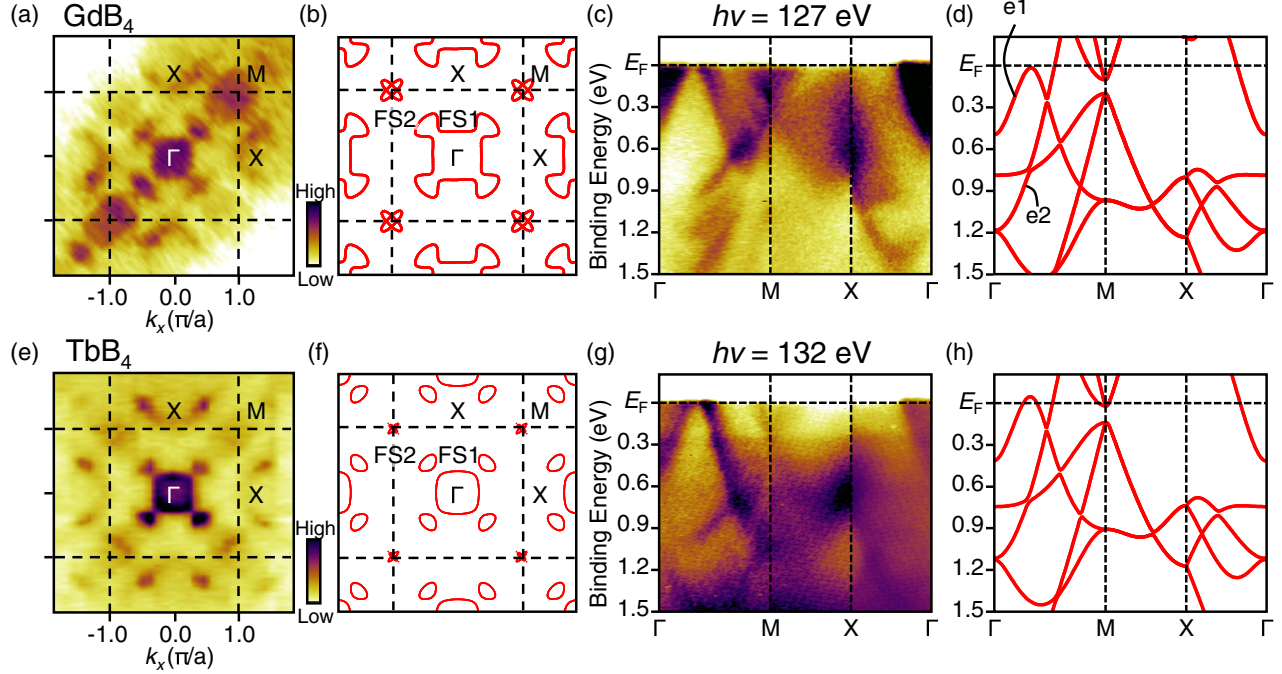


FIG. 2. (a) FS mapping of GdB₄ in the k_x - k_y plane at $k_z \sim 0$ obtained at $h\nu = 127$ eV. (b) Corresponding calculated Fermi surface. (c) ARPES intensity plot of GdB₄ in the $k_z = 0$ plane along Γ -M-X- Γ high-symmetry lines. (d) Corresponding calculated band dispersion. (e)–(h) Same as panels (a)–(d) but for TbB₄ ($h\nu = 132$ eV).

0.5 eV below E_F at the Γ point and 0.1 eV below E_F at the M point, respectively. These bands are primarily derived from B $2p$ orbitals. The anomalous elongation of FS1 along the Γ -M direction in Fig. 2(a), giving rise to the jigsaw-puzzle-like shape, is attributed to the backfolding between the Γ -centered electron band (denoted as e1) and another electron band with a minimum at about 1.2 eV (e2). A side-by-side comparison of the calculated band dispersions and the ARPES intensity along the Γ -M-X- Γ cut in Figs. 2(c) and 2(d) shows qualitative agreement, while some quantitative differences can be seen. These include a downward energy shift of the experimental electron band at the M point relative to the calculation, as well as a broad spectral intensity around the X point in the energy range of E_F –0.8 eV, where no corresponding bands are predicted by the calculations. We further find that the FS topology of TbB₄ is very similar to that of GdB₄, with only slight differences in FS volume, as shown in Figs. 2(e)–2(h). These results indicate that first-principles calculations provide a reasonable starting point for describing the experimental electronic structure of RB₄. In the following, we mostly focus on a more detailed analysis of the band dispersions in TbB₄, for which higher-quality ARPES data for nodal lines are available.

IV. NODAL-LINE ELECTRONIC STATES

Figure 3 shows theoretical and experimental band dispersions along a series of k cuts parallel to the k_x axis, which intersect the glide-mirror-invariant plane at $k_x = 1.0$ (in units of π/a) perpendicularly [dashed orange lines in Fig. 3(a)]. By systematically varying k_y from 0.0 (cut 1) to 1.0 (cut 11) at

$k_z = 0$, all cuts pass through the same XM line and the Dirac-like band crossings are expected to persist even under SOC. The first panel of Fig. 3(b) depicts the calculated band dispersion along cut 1 ($k_y = 0$, corresponding to the Γ -X line), which crosses the glide-mirror planes at $k_y = \pm 1.0$. Two bands in the energy range of 0.8–1.3 eV (orange curves, hereafter referred to as the P1 bands) intersect exactly at $k_x = 1.0$ at an energy of approximately 0.8 eV. Another pair of bands exhibits an analogous band crossing at a higher binding energy (E_B) of about 1.3 eV. As k_y is increased from cut 1 to cut 9, the crossing points remain pinned at $k_x = \pm 1.0$, independent of k_y , while their energies evolve continuously: The crossing point shifts upward for the P1 bands, accompanied by a substantial change in the band width. Notably, because the nodal lines are protected by glide-mirror symmetry, avoided crossings are forbidden on the glide-mirror plane. This symmetry protection is manifested experimentally as simultaneous band degeneracies for the P1 band (and also the other bands) at the glide-mirror-invariant momenta.

We now turn to the corresponding experimental ARPES data. We first focus on cut 5, taken at an intermediate momentum $k_y = 0.4$, shown in the middle panel of Fig. 3(c). Although the ARPES intensity is partially complicated by the overlap of the P1 and the other bands, an X-shaped dispersion associated with the P1 band can be clearly identified on both sides of the BZ, exhibiting a crossing point at $E_B \sim 0.9$ eV at $k_x = \pm 1.0$. To trace the Dirac-like band crossings, we performed a systematic analysis of the ARPES data based on MDCs over a wide energy range for multiple momentum cuts (see Appendix B for the analysis of full MDCs). The peak positions extracted from Lorentzian fits trace the experimental

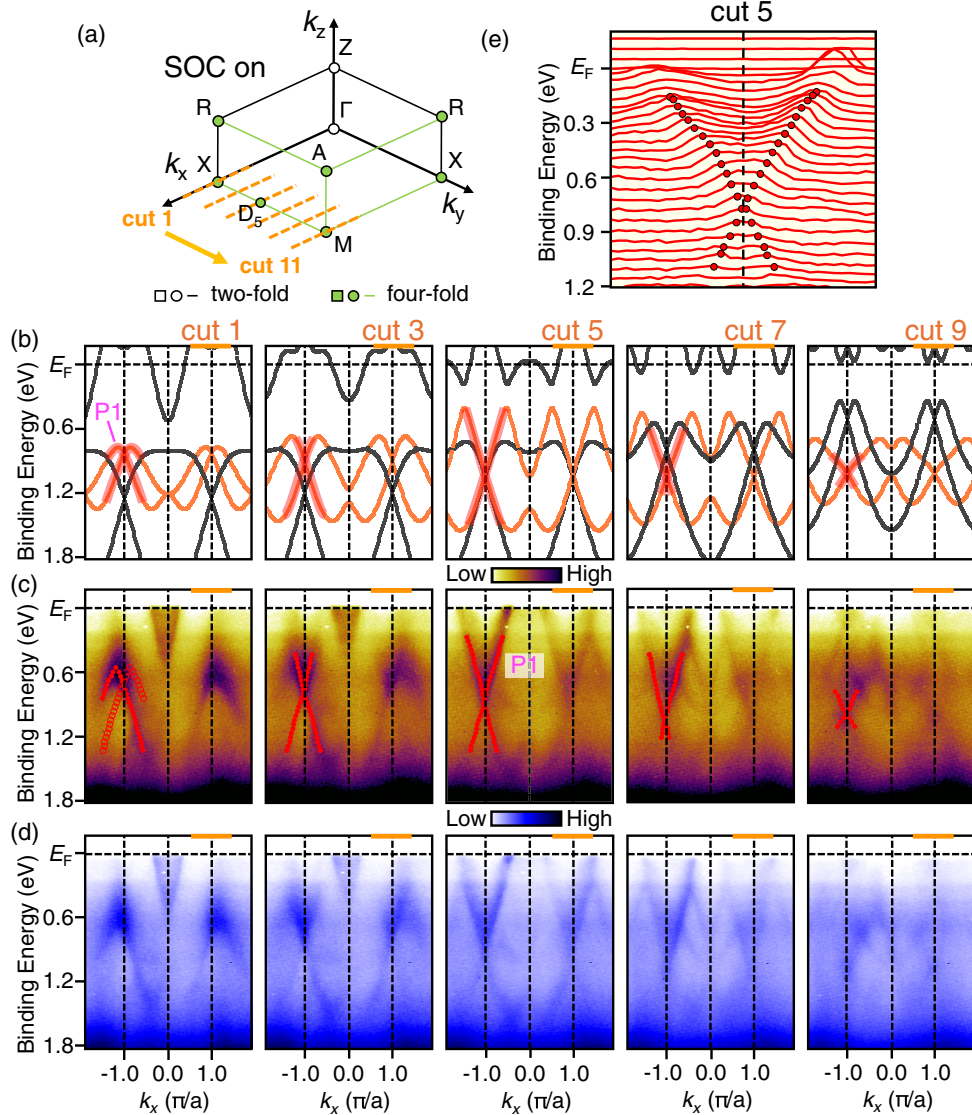


FIG. 3. (a) Tetragonal bulk BZ. Green lines show the k -regions where the energy bands exhibit fourfold degeneracy in the presence of SOC. k cuts (cuts 1–11) where the ARPES measurements were carried out are also indicated by dashed orange lines (note that the actual k range also covers negative k_x). (b) Calculated band dispersion and (c) ARPES intensity plot in the paramagnetic phase ($T = 50$ K) for TbB_4 obtained along cuts 1, 3, 5, 7, and 9 at $h\nu = 132$ eV. Red filled circles in panel (c) are the experimental band dispersion determined by analysis of the momentum distribution curves (MDCs) as shown in panel (e). Red open circles in the left panel are energy dispersions obtained by symmetrizing the filled circles with respect to the BZ boundary. The corresponding bands in the calculations are highlighted by orange and shaded red lines in panel (b). (d) Same as panel (c) but measured in the AFM phase ($T = 7$ K). (e) MDCs along cut 5.

band dispersions without relying on guides to the-eye. As shown in Fig. 3(c), the extracted dispersions exhibit clear X-shaped crossings over an extended energy window, which are already visible in the raw MDCs themselves [Figs. 7 and 3(e)]. Furthermore, the systematic evolution of the crossing point across different k cuts (cuts 1–9) shown in Fig. 3(c) indicates that the observed X-shaped dispersions arise from a continuous nodal-line feature in k space rather than accidental overlaps. While first-principles calculations assign the overall band topology and confirm the symmetry origin of the degeneracy, the systematic k dependence of the crossing points observed here provides experimental support for the nodal-line interpretation of the Brillouin-zone-boundary states.

We also examine the influence of magnetic order, by performing ARPES measurements at $T = 7$ K, well below the Néel temperature ($T_N \sim 44$ K). Although the AFM order is theoretically expected to break the glide-mirror symmetry and open a gap at the crossing points, the observed spectral features in Fig. 3(d) are not resolvable different from those in the PM phase [Fig. 3(c)]. Specifically, the band-crossing behavior is preserved within experimental resolution, with no discernible gap opening. We emphasize that this comparison cannot distinguish a genuine absence of magnetic-order effects on the nodal-line states from an AFM-induced modification too small to resolve with the present energy and angular resolution. We therefore do not inter-

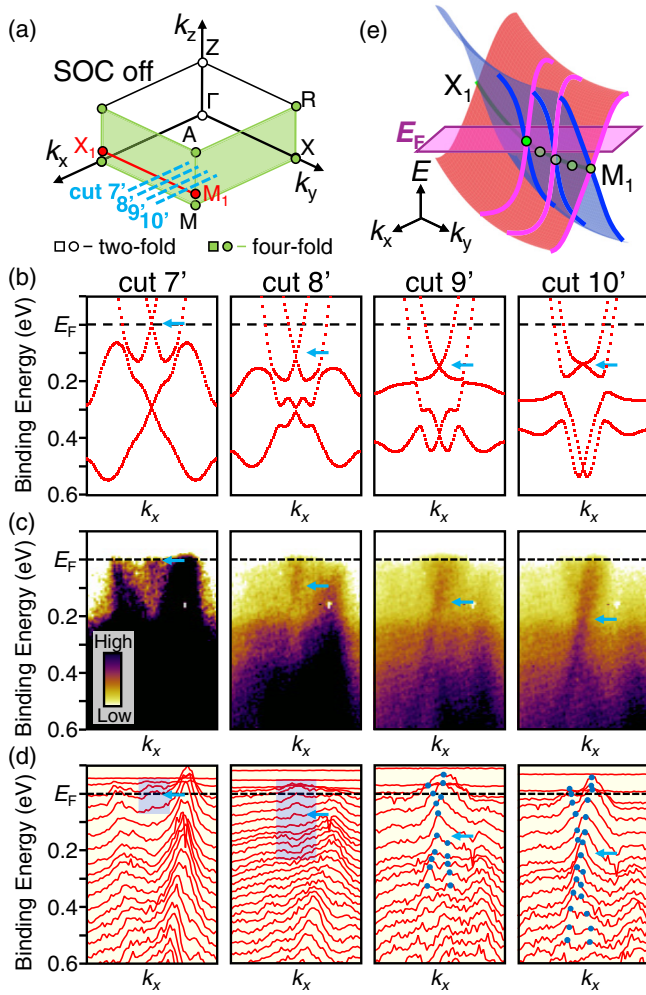


FIG. 4. (a) Tetragonal bulk BZ. Cuts 7'–10' are also indicated by dashed light blue lines. M_1X_1 cut is also indicated by a solid red line. (b) Calculated band structure along cuts 7'–10'. Light blue arrows indicate the band-crossing points. (c) Corresponding ARPES intensity plots. (d) Corresponding MDC plots in which blue circles in cuts 9' and 10' indicate the extracted peak positions, corresponding to the experimental band dispersions. The shaded areas in cuts 7' and 8' indicate the (E, k) region where the Dirac-like band exists. (e) Schematic illustration of the calculated Dirac-like dispersion along the M_1X_1 line, which approaches and crosses E_F in the calculation. We note that, although the same photon energy as in Fig. 2 was employed, the nodal line located slightly away from the $k_z = 0$ plane can be experimentally accessed owing to the finite k_z broadening.

pret this observation as establishing that the nodal-line states are robust against, or decoupled from, the magnetic order; clarifying this point will require a higher-resolution ARPES measurement in future work.

Having identified dispersions associated with glide-mirror-symmetry-enforced nodal lines, we next address whether such nodal lines can contribute to the electronic transport properties. To this end, we carefully examine the experimental band structure in the PM phase in the immediate vicinity of E_F and identify signatures of another nodal-line feature that crosses E_F . Figure 4(b) presents the calculated band dispersions along

a set of k cuts whose in-plane momenta (k_x and k_y) are identical to those of cuts 7–10 in Fig. 3(a), while the out-of-plane momentum is chosen slightly away from the $k_z = \pi$ plane, at $k_z = 0.125\pi$. These cuts are denoted as 7'–10' and are schematically illustrated in Fig. 4(a). Along cut 10', a crossing point is clearly resolved at a binding energy of $E_B \sim 0.2$ eV. Although this crossing at finite k_z is, in principle, fragile against SOC unlike the nodal line along the XM line shown in Fig. 3, the SOC-induced gap is extremely small in the present case due to the weak atomic SOC of the B-derived states. Indeed, the calculated SOC gap along these cuts is only in the range of 0.2–4.6 meV, and it can hardly be resolved with the present energy resolution. Upon moving the k cuts from 10' toward 7', the band-crossing feature shifts continuously upward in energy and eventually crosses E_F at cut 7'. In the corresponding ARPES intensity and MDC plots shown in Figs. 4(c) and 4(d), an X-shaped band dispersion crossing at $E_B \sim 0.2$ eV is clearly observed along cut 10', in good agreement with the calculation. While the lower branch of the Dirac dispersion exhibits a steeper dispersion in the experiment than in the calculation, the overall band topology is well reproduced. As the k cut approaches 7', the experimentally observed crossing point gradually moves upward and appears to cross E_F , consistent with the theoretical prediction.

The spectral feature of this E_F -crossing nodal line [see Fig. 4(e) for schematics] highlights its possible relevance to the transport properties of RB_4 . In particular, unusually large MR has been observed in a number of systems hosting SOC-robust or SOC-fragile nodal-line states, including the prototypical nodal-line semimetal $ZrSiS$ ($2 \times 10^4\%$) [12], as well as $PtSn_4$ ($1.55 \times 10^5\%$) [10], MoO_2 ($5 \times 10^4\%$) [65], $CaCdSn$ ($7.4 \times 10^3\%$) [13], and $Pd_3Ti_2S_2$ ($1.5 \times 10^4\%$) [66]. A notable commonality among these materials is that the nodal lines are located at or in close proximity to E_F . Such a band topology is often discussed as being favorable for high-mobility electronic transport and pronounced MR responses, although the microscopic mechanisms can be material dependent and remain under active investigation. In particular, multiple mechanisms—including carrier compensation, mobility imbalance, magnetic scattering, and field-induced Fermi-surface reconstruction—have been discussed in the literature.

Within the RB_4 family, GdB_4 has also been reported to exhibit a very large MR [67]. Given that GdB_4 and TbB_4 show experimentally very similar electronic structures, it is reasonable to consider that the nodal line crossing E_F may be relevant to the observed magnetotransport properties. To further clarify this point, we have analyzed the possible microscopic mechanisms based on the calculated electronic structure. In brief, the calculated three-dimensional Fermi surfaces indicate that the system is close to a compensated semimetal, providing a natural condition for large MR within a two-carrier framework. At the same time, the observed nodal-line features near E_F may offer favorable conditions for high carrier mobility. While other mechanisms such as magnetic scattering or field-induced Fermi-surface reconstruction cannot be completely excluded, they are not naturally consistent with the available experimental and theoretical considerations (Appendix C).

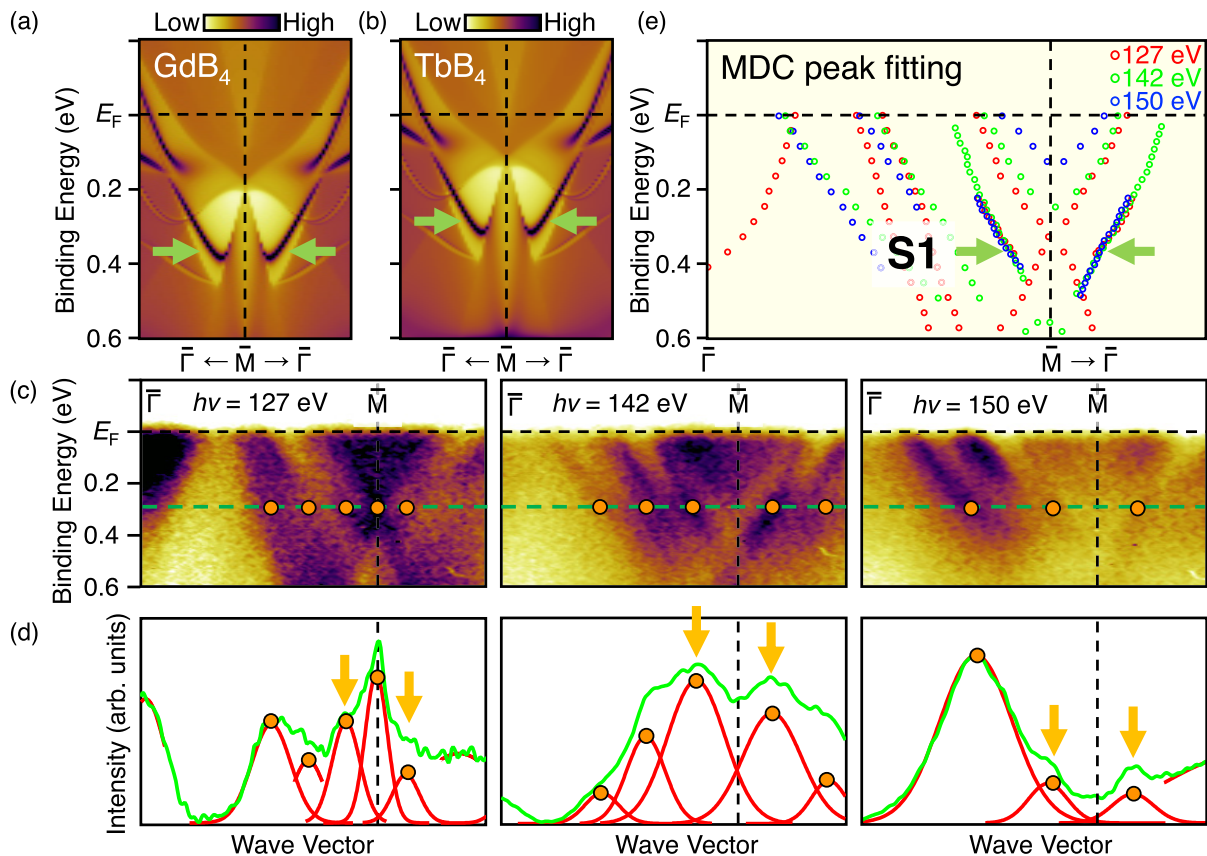


FIG. 5. (a) and (b) Surface band structure for the (001) semi-infinite slab calculated using the Green's function method for GdB_4 and TbB_4 , respectively. Surface states corresponding to the experiment are indicated by green arrows. (c) ARPES intensity plot along $\bar{M}$ - $\bar{\Gamma}$ line of the surface BZ for GdB_4 , obtained at the photon energies of $h\nu = 127, 142$, and 150 eV. (d) MDCs (green curves) along the dashed green line in panel (c), together with the result of numerical fitting using multiple Lorentzians (red curves). Orange circles represent peak positions. (e) Experimental band dispersion obtained by tracing the peak position of the MDCs with the numerical fittings. Surface-related band dispersion that was identified by the $h\nu$ independence is also indicated by green arrows.

V. SURFACE STATES AND BULK TOPOLOGY

Beyond their relevance to transport, the topological nature of these nodal lines is of fundamental importance, as a nontrivial Berry phase is essential for the emergence of boundary electronic states. Since the standard characterization via the Zak phase [1,3,5,21] is hindered by the open trajectories of the nodal lines constrained to the BZ boundaries, we instead evaluate the Berry phase (θ) along closed k -loops encircling the XM line at various k_x values (corresponding to cuts 1–11). To provide a gauge-consistent topological diagnosis even in the presence of band degeneracies, we formulate the topological invariant in terms of the Wilson loop (non-Abelian Berry phase; see Appendix D) [68–70]. On the $k_x = 0$ plane, where the Hamiltonian commutes with the glide-mirror operator, the Hilbert space can be decomposed into independent glide sectors. Within each sector, the Berry phase evaluated along loops encircling the nodal line is quantized to $\pi \pmod{2\pi}$, demonstrating the nontrivial topology [50,71]. For planes away from $k_x = 0$, the glide-sector decomposition is no longer applicable. We therefore compute the Wilson-loop matrix and examine its eigenvalues. For such paths, small deviations from exact quantization are observed. Nevertheless, the fact that

the Wilson-loop eigenvalues remain close to $\pm\pi$ suggests that the nontrivial topological character persists, at least approximately, in the vicinity of the nodal line.

The nontrivial topological character of the nodal line is expected to give rise to surface states. We examined the surface electronic structure using spectral-intensity calculations for a semi-infinite (001) slab based on the Green's function method. As shown in Figs. 5(a) and 5(b), first-principles calculations predict SS weight along the $\bar{M}$ - $\bar{\Gamma}$ cut of the surface BZ for both GdB_4 and TbB_4 . The SS exhibits a characteristic W-shaped dispersion near the edge of the projected bulk bands and is connected to the projection of the bulk nodal line located at $E_B \sim 0.2$ eV at the $\bar{M}$ point. We note that the calculated surface electronic structures for GdB_4 and TbB_4 are essentially identical in this (E, k) region, supporting the robustness of the present interpretation.

To experimentally probe these SS, we performed ARPES measurements along the same $\bar{M}$ - $\bar{\Gamma}$ cut using three different photon energies (127, 142, and 150 eV) as shown in Fig. 5(c). Figure 5(d) displays the corresponding MDCs taken at $E_B = 0.3$ eV along the dashed green line in Fig. 5(c). At $h\nu = 127$ eV, an X-shaped band centered at the $\bar{M}$ point is clearly

observed. With increasing photon energy, the upper branch becomes disconnected from the lower branch at $h\nu = 142$ eV and shifts further upward at $h\nu = 150$ eV, indicating a bulk origin associated with finite k_z dispersion. In addition to these bulk-derived features, we identify another broader V-shaped band whose energy position remains essentially unchanged upon varying $h\nu$. To quantitatively track the band dispersions, we performed Lorentzian fits to the MDCs and summarize the resulting dispersions in Fig. 5(e). While most bands exhibit clear photon-energy dependence, one band remains nearly unchanged and is therefore assigned as a surface-related origin and labeled S1, in good agreement with the slab calculations in Figs. 5(a) and 5(b). We note that part of the Λ -shaped component of the W-shaped SS predicted by the calculation may merge into the bulk band edge, which could account for its reduced visibility in the experiment. The energy-momentum region of this experimentally identified SS is consistent with the calculated surface spectral function associated with the nontrivial π Berry phase of the bulk nodal line. We note, however, that photon-energy independence alone cannot distinguish a topological surface state from a trivial surface state or a surface resonance, so this observation does not by itself establish the topological origin of the SS.

The discovery of nonsymmorphic-enforced nodal lines in RB_4 opens up several exciting avenues for future research. First, given that the RB_4 family exhibits a variety of magnetic ground states arising from the Shastry-Sutherland lattice, our findings suggest that these topological states may be a universal feature across the series [64,72–74]. This provides a fertile ground to explore the interplay between topological fermions and exotic magnetism, such as fractional magnetization plateaus [74–78]. The absence of a pronounced reconstruction across the antiferromagnetic transition within the present experimental sensitivity motivates higher-resolution studies to determine whether the nodal-line-related electronic structure remains gapless or undergoes subtle modifications in different magnetic phases. Such studies may also clarify the possible consequences of these states for quantum transport signatures and potential correlation effects [79–82]. Consequently, the RB_4 family provides a promising platform for studying the coexistence and possible coupling of nonsymmorphic nodal-line electronic states and frustrated magnetism.

VI. CONCLUSION

In conclusion, we have investigated the electronic structure of rare-earth tetraborides RB_4 ($R = \text{Tb, Gd}$) using microfocused ARPES and first-principles calculations. ARPES reveals systematically evolving Dirac-like dispersions along the Brillouin-zone boundaries in the paramagnetic phase, supporting their assignment to the nonsymmorphic nodal lines enforced by the crystal symmetry. Near E_F , the observed dispersive features follow the calculated nodal-line-derived band structure, although the exact crossings and the predicted few-meV SOC gaps are not resolved experimentally. Photon-energy-dependent ARPES further identifies a surface-related feature whose dispersion is consistent with the calculated surface spectral function, while Wilson-loop calculations establish the nontrivial topology of the corresponding calculated bulk bands under the relevant symmetry conditions. No pro-

nounced reconstruction of the nodal-line-related dispersions is resolved across the antiferromagnetic transition. These results provide an ARPES-based characterization of nonsymmorphic nodal-line electronic structures in magnetic rare-earth tetraborides, supported by symmetry and first-principles analyses, and motivate further high-resolution studies of their relation to magnetism and transport.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

APPENDIX A: THREE-DIMENSIONAL ELECTRONIC STRUCTURE OF GdB_4 AND TbB_4

To establish the three-dimensional bulk electronic structure of GdB_4 and TbB_4 , we performed normal-emission ARPES measurements, in which the out-of-plane momentum k_z was tuned by varying the photon energy. The resulting three-dimensional electronic structure is shown in Figs. 6(a) and 6(b) as E_F intensity maps plotted as a function of k_x and k_z for GdB_4 and TbB_4 , respectively. The observed intensity exhibits a clear periodic modulation along the k_z direction, demonstrating that the measurements probe bulk electronic states. By comparing these results with the calculated band structure, the high-symmetry points Γ and Z can be consistently assigned, as indicated in Figs. 6(a) and 6(b). This periodicity provides a reliable basis for converting photon energy to out-of-plane momentum. From the observed k_z periodicity, the inner potentials V_0 were determined to be 27 eV for GdB_4 and 23 eV for TbB_4 . Using these values, the ARPES intensity for GdB_4 was converted into an energy- k map as a function of binding energy E_B and k_z , as shown in Fig. 6(c). The overall agreement between experiment and calculation (red curves) is reasonable: Electronlike states centered at the Γ point, holelike states with band maxima at approximately 1 eV binding energy near the Γ point, and holelike states with maxima around 2 eV at the Z point are all consistently reproduced.

APPENDIX B: MDC-BASED EXTRACTION OF BAND DISPERSIONS

To quantitatively track the band dispersions observed in the ARPES data in Fig. 3(c), we perform a systematic anal-

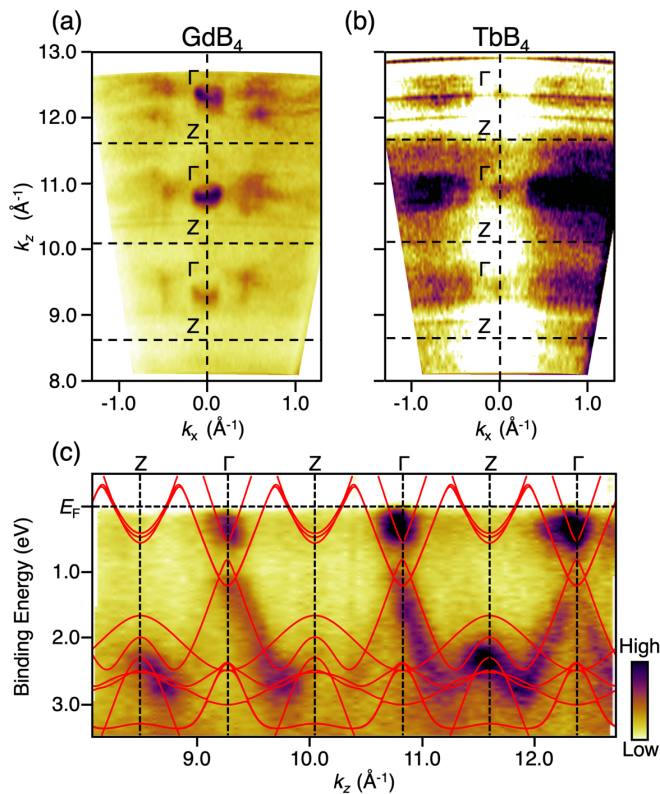


FIG. 6. (a) and (b) ARPES intensity mapping at E_F in the k_x - k_z plane for GdB_4 and TbB_4 , respectively, obtained with SX photons. (c) ARPES intensity plot along the Γ -Z cut obtained from normal-emission measurements for GdB_4 . The red curves represent the calculated band structure.

ysis based on MDCs. Figure 7 shows representative MDCs taken over a wide energy range for selected k cuts. The peak positions are extracted by fitting the MDCs with Lorentzian functions. Only well-defined peaks associated with the nodal lines are considered in the analysis, and no guides to the eye are introduced. The resulting peak positions (filled circles) trace the experimentally resolved dispersions, which exhibit clear X-shaped dispersive features over an extended energy window, consistently observed across multiple k cuts and already visible in the raw MDC data.

This systematic evolution across k cuts supports the assignment of these features to the nonsymmorphic-symmetry-enforced nodal line at the Brillouin-zone boundary. We apply

the same MDC-based approach to the data near E_F [Fig. 4(d)]; owing to the increased spectral linewidth in this region, individual branches cannot always be reliably decomposed, but the extracted peak positions approach the energy-momentum region of the crossing predicted by the calculations. We therefore assign the near- E_F features to nodal-line-derived states on the basis of the combined MDC analysis, symmetry considerations, and first-principles calculations, rather than on the ARPES data alone.

APPENDIX C: CARRIER COMPENSATION AND POSSIBLE MECHANISMS FOR LARGE MAGNETORESISTANCE

We discuss possible mechanisms underlying the large MR observed in this material family, based on the electronic structure obtained from first-principles calculations. We first consider carrier compensation and mobility imbalance. Using the three-dimensional Fermi surfaces obtained from the calculations for bulk GdB_4 in the nonmagnetic phase, we quantitatively evaluate the carrier type and carrier density associated with each Fermi-surface sheet. The results are summarized in Fig. 8. We find that the total carrier densities of holes and electrons are nearly balanced, with $n_h \approx 8.22 \times 10^{20} \text{ cm}^{-3}$ and $n_e \approx 7.61 \times 10^{20} \text{ cm}^{-3}$, indicating that GdB_4 is close to a compensated semimetal. This provides a quantitative basis for considering carrier compensation as a contributing factor to the large MR. Within a compensated two-carrier framework, the magnetoresistance is expected to scale as $\text{MR} = \mu_e \mu_h B^2$, where μ_e and μ_h denote the electron and hole mobilities, respectively. This relation implies that a large MR additionally requires high carrier mobility. In this context, the presence of nodal lines near E_F may provide favorable conditions for enhanced mobility and thus could contribute to the observed MR. At the same time, we emphasize that the present study does not include direct transport measurements and therefore does not uniquely establish the microscopic origin of the MR.

We next consider magnetic scattering. While spin-disorder scattering can contribute to MR, such a mechanism typically leads to a tendency toward saturation at high magnetic fields due to the suppression of spin fluctuations. This behavior is not naturally consistent with the large, nonsaturating MR reported for this material family. Finally, we examine the possibility of field-induced Fermi-surface reconstruction, which was proposed by Shon *et al.* [67]. While we cannot rule out

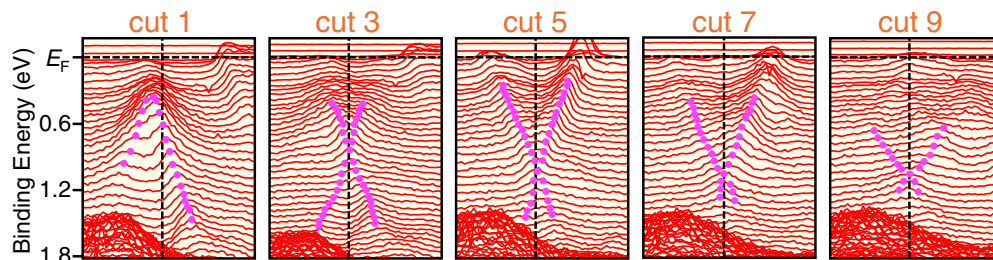


FIG. 7. MDCs along cuts 1, 3, 5, 7, and 9 in the negative k_x region of Fig. 3(c) for TbB_4 . Filled circles indicate the extracted peak positions corresponding to experimental band dispersions. Only well-resolved peaks are used, and no guides to the eye are introduced, ensuring that the extracted dispersions directly reflect experimental observables.

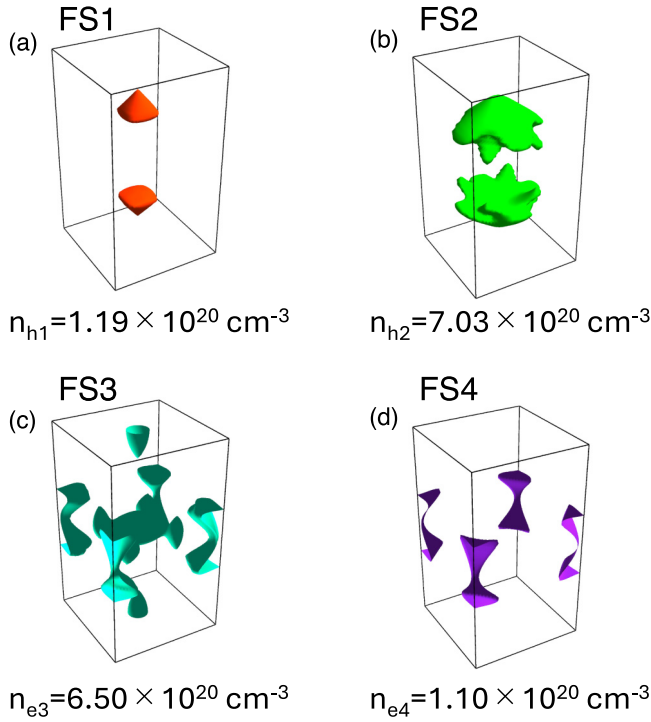


FIG. 8. (a) Calculated Fermi surfaces of GdBi_4 in the nonmagnetic phase within the three-dimensional Brillouin zone. Carrier types (hole or electron) and carrier densities are also indicated.

such a scenario, in the present system the characteristic energy scale associated with the applied magnetic field is much smaller than the electronic bandwidth. Moreover, the experimental and calculated Fermi surfaces are large enough that they are expected to remain insensitive to the applied magnetic field over most of the Brillouin zone. These considerations suggest that substantial field-induced modifications of the Fermi-surface topology are unlikely, and this mechanism is not expected to play a dominant role. A direct assessment of this mechanism would require field-dependent band-structure calculations or spectroscopic measurements under magnetic

field, which lie beyond the scope of the present study. Taken together, these considerations lead us to regard carrier compensation combined with high carrier mobility as a plausible band-structure-related contributing factor to the large magnetoresistance in this system, alongside other mechanisms that cannot be fully excluded. As noted above, the present study does not include direct transport measurements, and we therefore do not claim to establish a unique microscopic origin of the MR.

APPENDIX D: BERRY-PHASE ANALYSIS OF NODAL-LINE STATES

We formulate the topological invariant in terms of the Wilson loop (non-Abelian Berry phase), which provides a gauge-consistent framework for evaluating the Berry phase even in the presence of band degeneracies [68–70]. On the $k_x = 0$ plane, where the Hamiltonian H commutes with the glide-mirror operator G_x and each Kramers pair carries opposite G_x eigenvalues, we decompose the Hilbert space into two glide sectors (g_+ and g_-) and evaluate the Berry phase independently within each sector along closed loops encircling the nodal line [see Fig. 9(b)]. For planes away from $k_x = 0$, the glide-sector decomposition is no longer applicable. We therefore compute the Wilson-loop matrix W_C and its eigenvalues for the two-band subspace rather than evaluating the Berry phase of each band separately:

$$W_C = \mathcal{P} \exp \left[i \oint_C \mathbf{A}(\mathbf{k}) \cdot d\mathbf{k} \right]. \quad (\text{D1})$$

Here, $\mathbf{A}(\mathbf{k})$ is the Berry connection matrix defined as $[\mathbf{A}(\mathbf{k})]_{mn} = i \langle u_{m\mathbf{k}} | \nabla_{\mathbf{k}} u_{n\mathbf{k}} \rangle$ and $\mathcal{P}$ denotes the path ordering. This approach provides a gauge-consistent generalization of the Berry phase for a path encircling band-degenerate points within the enclosed region. As summarized in Fig. 9(c), the Berry-phase values for paths on the $k_x = 0$ plane are quantized to $\pm\pi \pmod{2\pi}$, confirming the nontrivial topology of the nodal-line states. For paths 3–9 away from this plane, small deviations from exact quantization are observed; we attribute these, at least in part, to the fact that the bands associated

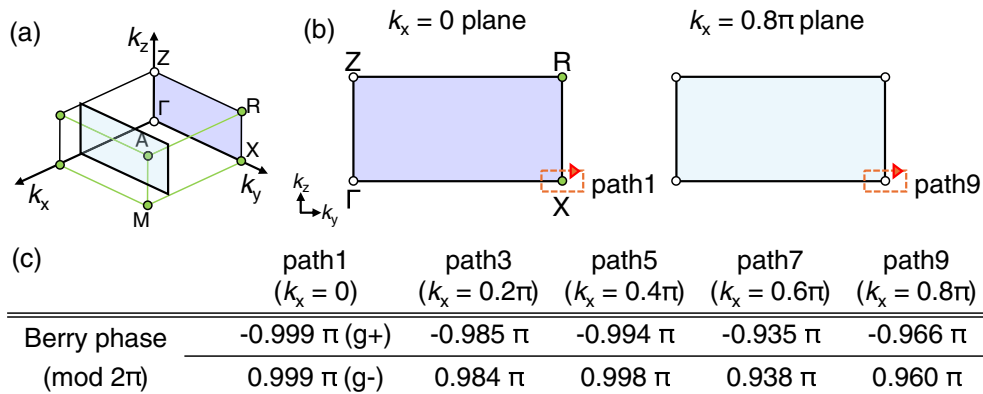


FIG. 9. (a) Three-dimensional Brillouin zone indicating the high-symmetry points and the planes used for the Berry-phase evaluation. (b) Schematic illustration of closed momentum-space paths encircling the nodal line on the $k_x = 0$ plane (left) and on a representative off-symmetry plane ($k_x = 0.4\pi$, right). (c) Table of Berry-phase-related quantities (mod 2π) calculated along these paths. On the $k_x = 0$ plane, the values represent the Berry phase evaluated independently in the glide eigenvalue sectors (g_+ and g_-). For planes away from $k_x = 0$, the values represent the eigenvalues of the Wilson-loop matrix computed for the degenerate two-band subspace.

with the nodal line may cross or hybridize along intermediate paths, making the encirclement of a single nodal line less well defined. Nevertheless, the fact that the Wilson-loop eigenvalues remain close to $\pm\pi$ even for paths away from the $k_x = 0$ plane suggests that the nontrivial topological char-

acter persists, at least approximately, in the vicinity of the nodal line. These results indicate that the nodal-line states on the Brillouin-zone boundary are characterized by a nontrivial Berry phase protected by glide symmetry, providing a consistent topological diagnosis of the open nodal line.

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