Drumhead surface states and their signatures in quasiparticle scattering interference

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We consider a two-orbital tight-binding model defined on a layered three-dimensional hexagonal lattice to investigate the properties of topological nodal lines and their associated drumhead surface states. We examine these surface states in centrosymmetric systems, where the bulk nodal lines are of Dirac type (i.e., four-fold degenerate), as well as in non-centrosymmetric systems with strong Rashba and/or Dresselhaus spin-orbit coupling, where the bulk nodal lines are of Weyl type (i.e., two-fold degenerate). We find that in non-centrosymmetric systems the nodal lines and their corresponding drumhead surface states are fully spin polarized due to spin-orbit coupling. We show that unique signatures of the topologically nontrivial drumhead surface states can be measured by means of quasiparticle scattering interference, which we compute for both Dirac and Weyl nodal line semimetals.

I. INTRODUCTION

The discovery of time-reversal invariant topological insulating materials with strong spin-orbit coupling (SOC) triggered an enormous research interest in decoding the topological phases of matter \cite{1–3}. One of the most important characteristics of topological materials is the existence of symmetry-protected metallic modes at the surface of the material, while the bulk shows insulating or semi-metallic behaviour. This property originates from the topologically nontrivial ordering of bulk wave functions and is characterized by a band inversion involving switching of bands of opposite parity around the Fermi level \cite{4, 5}. The recent theoretical prediction and experimental observation of topological nodal-line semimetals \cite{6–19}, Weyl semimetals \cite{20–30}, and Dirac semimetals \cite{31–43} has redirected the research interest from insulating topological materials to topological semimetals in the field of quantum condensed matter physics.

The defining feature of topological semimetals is the crossing of the conduction and the valence bands in the Brillouin zone (BZ) near the Fermi energy. These crossings are topologically protected against gap opening by any perturbation that preserves a certain symmetry group. These bulk band degeneracies can occur at discrete nodal-points or continuous nodal-lines resulting in zero-dimensional bulk nodal-points (Weyl/Dirac semimetals) or one-dimensional bulk nodal-lines (topological nodal-line semimetals). Weyl semimetals can be realized when either time reversal or inversion symmetry is broken, while the stability of Dirac nodal lines is guaranteed by time-reversal symmetry combined with inversion symmetry or a crystal symmetry, such as rotation or reflection. Therefore, a nodal line can either evolve from a crossing of two bands or two doubly degenerate bands, thus exhibiting Weyl character or Dirac character. In the following we call these two cases Weyl nodal-line semimetal (WNLS) and Dirac nodal-line semimetal (DNLS). In the Dirac and Weyl topological semimetallic states, the low-energy excitations are linearly dispersing Dirac and Weyl fermions. In WNLSs and DNLSs, on the other hand, the Weyl/Dirac fermions are linearly dispersing in only two momentum directions, while they are non-dispersive in the third direction, i.e., along the nodal line.

A nodal line which closes inside the BZ forming a nodal loop and carrying a topological charge, is associated with drumhead-like surface states \cite{3, 44–47}. These surface states are bounded by the projection of the nodal ring onto the surface, a region looking like the head of an open drum and hence are called drumhead surface states. Thus, the intricate interplay between symmetry and topology of the electronic wave functions gives rise to the associated two-dimensional drumhead-like surface states in topological nodal-line semimetals. Topological nodal-line semimetals exhibiting line-node bulk states and associated drumhead surface states present a signif-

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FIG. 1. Crystal structure of the three-dimensional layered system as viewed from the [001] (left panel) and the [010] (right panel) directions of the hexagonal lattice. Layer 1 (with B&C atoms) intercalates between the adjacent 2 layers such that A atoms are aligned with the B atoms in the z-direction.
FIG. 2. Upper panel: Bulk energy dispersion at $k_z=0$ along high symmetry lines in the BZ for (a) the Dirac nodal line semimetal, (b) the Weyl nodal line semimetal with pure Rashba ($\alpha = 0.2, \beta = 0.0$) or Dresselhaus ($\alpha = 0.0, \beta = 0.2$) SOCs, and (c) the Weyl nodal line semimetal with mixed Rashba and Dresselhaus ($\alpha = \beta = 0.1$) SOC. Here and in the rest of the paper, energies are measured in units of $t$. Lower panel: Energy dispersion of the surface density of states as a function of energy and momentum along high symmetry lines in the BZ for (d) the Dirac nodal line semimetal, (e) the Weyl nodal line semimetal (WNLS) with pure Rashba SOC (or pure Dresselhaus SOC), and (f) the WNLS with mixed Rashba and Dresselhaus SOC.

 significant expansion of topological materials beyond topological insulators and nodal point semimetals. They provide new opportunities to explore the exotic physics of topological materials. The novel properties of topological nodal-line semimetals, like drumhead surface states [41, 48–50], have opened new possibilities in high-$T_C$ superconductivity [10, 45, 51–55] and magnetic order [56], unique Landau energy levels [57], collective modes from the novel nodal line structure [58], and anomalies in electromagnetic and transport response [44, 59–67].

Many nodal line materials have been experimentally realized recently, like PbTaSe$_2$ [6], Ca$_3$P$_2$ [9, 68] CaAgP and CaAgAs [16, 42, 69–71]. Other candidate materials include TiTaSe$_2$ [7], fcc alkaline earth metals [72], hyperhoneycomb lattices [73] and the CaP$_3$ family [74]. Noncentrosymmetric PbTaSe$_2$ [10] and TiTaSe$_2$ [7] have reflection symmetry at the Ta atomic plane but lack inversion symmetry, and hence exhibit Weyl rings with two-fold degeneracy, while fcc alkaline earth metals, hyperhoneycomb lattices and Ca$_3$P$_2$ are protected by both inversion and time-reversal symmetry, and thus display Dirac rings which are four-fold degenerate. The noncentrosymmetric hexagonal ternary pnictides, CaAgP, CaAgAs, and SrPtAs are particularly promising candidates, since they can be grown in single crystal form [69–71, 75–79].

In this paper, we consider a two-orbital tight-binding model to study the topological properties of a three-dimensional layered hexagonal semimetal with both time-reversal and reflection symmetries. We study the effects of the presence and absence of inversion symmetry on the electronic band structure and topology of the surface states. In particular, we examine how Rashba and Dresselhaus spin-orbit couplings modify the properties of the nodal line and the drumhead surface states.

Furthermore, we compute the quasiparticle interference (QPI) patterns for both Dirac and Weyl nodal-line semi-metals and identify the signature of the drumhead surface states in these QPI patterns.

II. MODEL

In this section, we survey the topology of the band structure in a nodal line semimetal by means of a tight-binding model with two orbitals. These two orbitals form particle- and hole-like bands, which cross each other, generating a line-like degeneracy that is topologically protected. We consider two different scenarios with and without antisymmetric spin-orbit coupling (SOC), describing Weyl and Dirac nodal line semimetals, respectively. Our system consists of consecutive two-dimensional hexagonal layers of $s$ and $p_z$ orbitals, which are invariant under reflection symmetry ($R_z$) along the $z$-direction. Thus, the bands that cross near the Fermi energy have opposite $R_z$ symmetry eigenvalues, which prevents hybridization, keeping the line nodes in semimetals stable against gap opening. Fig. 1 shows the crystal
structure for this kind of system with lattice parameters $a$ and $c$. The orbitals of the tight binding model are located at sites $A$ and $B$, while the C-atoms break inversion symmetry. Our model can be assumed as a general description for the realization of topological drumhead surface states in a DNLSs like CaAgP and CaAgAs, as well as, WNLSs such as the ternary chalcogenides TiTaSe$_2$ and PbTaSe$_2$. In the latter ones, the nodal line lies in the $k_z = \pm \pi$ plane and closes around the $H$ point of the hexagonal BZ. The relevant orbitals there are $d$ and $p_{x,y}$, and the different symmetry eigenvalues come from the factor $e^{ik_z/2}$ for the atom located $c/2$ above the origin.

A. Dirac nodal line semimetal

We begin our analysis by discussing the Dirac nodal line semimetals which are invariant under both time-reversal and spatial inversion symmetry. This implies that both external magnetic field and antisymmetric SOC are absent. Without antisymmetric SOC the particle- and hole-like bands are spin-degenerate. Time-reversal, inversion, and $SU(2)$ spin-rotation symmetry together with a non-trivial band topology lead to a protected four-fold degenerate band crossing, which forms a nodal ring [9]. Based on this picture, we consider a spinless two-orbital tight-binding model with the Hamiltonian

$$
H_0 = \mu \sum_{i,\gamma \gamma'} \hat{\tau}_z \gamma' \gamma c_{i,\gamma}^\dagger c_{i,\gamma'} - \sum_{ij\gamma \gamma'} \left[ (t_{ij} \hat{\tau}_x \gamma' \gamma) c_{i,\gamma}^\dagger c_{j,\gamma'} + h.c. \right],
$$

(1)

where $c_{i,\gamma}^\dagger$ ($c_{i,\gamma}$) is the creation (annihilation) operator for an electron on site $i$ and orbital $\gamma$ ($= p, d$). Here, $t_{ij}$ and $t'_{ij}$ denote intra- and inter-orbital hopping amplitudes. Intra-orbital hopping is both, out of plane between first neighbours and in-plane between second neighbours, parametrized by $t_{\perp}$ and $t_{\parallel}$. Inter-orbital hopping is in between the layers and parametrized by $t'$. Moreover, $\hat{\tau}_i$ ($i = x, y, z$) are the Pauli matrices in orbital space and $\mu$ is an on-site energy, with opposite sign for $p$ and $d$ orbitals. For the numerical calculations, we set the values of the physical parameters to $(\mu, t_{\parallel}, t_{\perp}, t') = (3, 0.6, 1, 0.5)$. In momentum space, the Hamiltonian in Eq. (1) is given by

$$
H_0 = \sum_{k,\gamma \gamma'} \left[ \varepsilon_1(k) \hat{\tau}_z \gamma' \gamma + \varepsilon_2(k) \hat{\tau}_y \gamma' \gamma \right] c_{k,\gamma}^\dagger c_{k,\gamma'},
$$

(2a)

where

$$
\varepsilon_1(k) = \mu - 2t_{\perp} \cos(k_x c)
$$

(2b)

$$
\varepsilon_2(k) = -2t' \sin(k_z c/2).
$$

(2c)

Figure 2(a) shows the energy dispersion of Hamiltonian (2) along the KΓM path within the $k_z = 0$ plane of the BZ, which is invariant under $R_z$. It can be seen that around the $\Gamma$ point, two two-fold degenerate hole-and electron-pockets cross each other, generating a four-fold degenerate Dirac nodal ring. Figure 4(a) depicts the whole Dirac nodal ring at the $k_z = 0$ plane in the hexagonal BZ.

The Berry phase picked up by a closed path is $\pi$ whenever the nodal line is encircled and zero otherwise, showing the topological charge of the nodal line. We show the Berry phase calculated along $k_z$ in Fig. 3(a). More details on the calculation of the Berry phase are presented in Appendix B.

Now we show that the nontrivial topology of this nodal ring manifests itself as a so called drumhead surface state. For this purpose, we consider the system as a bundle of parallel two-dimensional $xy$-slabs ($n = 1, 2, ..., N_z$) piled upon one another in the $z$-direction. The boundary condition is periodic on each slab and open along the $z$-direction. Using the partial Fourier transformation $c_{k,\gamma}^\dagger = \frac{1}{N_z} \sum_{n} e^{i k_z a n} c_{k,\gamma}^\dagger$, with $k_\parallel = (k_x, k_y)$, the bulk BZ will be mapped into the slab geometry configuration on the new basis $\Phi_{n,k_\parallel}^\dagger = (c_{n,k_\parallel,d}, c_{n,k_\parallel,p})$, by the boundary condition $\Phi_{0,k_\parallel} = \Phi_{N_z-1,k_\parallel} = 0$ within the two-orbital model, and $n = 1, ..., N_z$. In this basis the Hamiltonian is given by [80, 81]

$$
H_{k_\parallel} = \sum_{n=0}^{N_z} \Phi_{n,k_\parallel}^\dagger \left( T \Phi_{n-1,k_\parallel} + M \Phi_{n,k_\parallel} + T^\dagger \Phi_{n+1,k_\parallel} \right).
$$

(3)

The hopping matrix $T$ connects two consecutive slabs, while $M$ contains hopping terms within a slab as well as on-site energies. Both the intra- and inter-orbital contributions are present in the hopping matrices $T$ and $M$,
FIG. 4. Momentum dependency of the spectral functions and their spin polarizations for drumhead surface states. (a-c) Bulk Fermi surfaces within the $k_z = 0$ correspond to the nodal rings. The subplots (d-f) show the momentum-resolved surface density of states $\rho_{n=1}(k_\parallel, \omega = 0)$. The solid lines indicate the first BZ. In the first two rows, the left, middle and right rows represent (a,d) a DNLS, (b,e) a WNLS with pure Rashba/Dresselhaus, and (c,f) a WNLS with the same strengths of Rashba and Dresselhaus SOCs, respectively. The third and fourth rows indicate the $x$- and $y$- components of the spin-resolved surface spectral function $\rho_{n=1}(k_\parallel, \omega = 0)$ for the WNLS with (g,j) Rashba, (h,k) Dresselhaus, and (i,l) mixed SOC. The labels are $(k_x, k_y)$ with units of $\pi/a$. 

which are given by:

$$M = \tilde{\varepsilon}_1(k_\parallel)\tau_z = -t'\tau_z;$$

$$T = -t_\perp \tau_z - \frac{1}{2}t'(\tau_x - i\tau_y).$$  \hspace{1cm} (4)

Here $\tilde{\varepsilon}_1$ is given by Eq. (2b), but without the $k_z$ dependent terms.

For $k_\parallel$ within the projected nodal ring, there is a band inversion and there are surface bound states among the eigenstates of the slab Hamiltonian (3), which decay exponentially along the $z$-direction into the bulk. These surface states are a manifestation of the topological properties of the system. To reveal these surface states it is useful to compute the local density of states (LDOS), $N_n(\omega)$, for a given slab $n$. The LDOS is computed by use of the Matsubara and retarded Green’s functions, which are defined for the slab geometry as

$$\hat{G}(k_\parallel, i\omega) = (i\omega - \mathcal{H}_{k_\parallel})^{-1}$$

and $\hat{G}_{\text{ret}}(k_\parallel, \omega) = \hat{G}(k_\parallel, i\omega \to \omega + i0^+)$. With this, the LDOS for the $n$th slab is obtained as

$$N_n(\omega) = -\frac{1}{\pi} \sum_{k_\parallel} \text{Im} \left[ \text{Tr} \left[ \hat{G}_{\text{ret}}(k_\parallel, \omega) \right] \right],$$  \hspace{1cm} (5)

and the momentum-resolved LDOS reads

$$\rho_n(k_\parallel, \omega) = -2 \text{Im} \left[ \text{Tr} \left[ \hat{G}_{\text{ret}}^{\text{mn}}(k_\parallel, \omega) \right] \right],$$  \hspace{1cm} (6)

where the trace runs over orbital and spin degrees of freedom. In Fig. 2(d) we present the momentum-resolved spectral function (momentum-resolved density of states) for the surface slab of the DNLS along high-symmetry lines in the BZ. This reveals the formation of topological surface states around the $\Gamma$ point, in the interior of the bulk Dirac nodal ring. Indeed, the surface modes can be easily observed as an in-gap drumhead surface state in the momentum-resolved spectral function of the surface slab inside the hexagonal BZ [see Fig. 4(d)]. These two-dimensional drumhead surface states are bounded by the projection of the one-dimensional bulk Dirac nodal ring onto the surface. Fig. 3(b) shows the $k$-integrated LDOS of the surface layer. While a nodal line semimetal has a vanishing DOS at Fermi level in the bulk, the surface states contribute to a non-vanishing value. The energy range of their dispersion is marked by Van Hove singularities.

Quasiparticle interference (QPI) is an efficient tool to observe topological surface states in different classes of topological materials [82, 83]. It can provide useful information about the topological properties of the surface.

FIG. 5. QPI patterns for the spinless case at different bias $\omega = -0.5, 0.0$ and $+0.5$. The axis in the color plot are $(q_x, q_y)$ in units of $\pi/a$. The lower plot shows a cut along the dashed line.
electronic band structure. QPI patterns can be experimentally obtained from the Fourier transformation of spatially modulated STM data, due to the elastic scattering of quasiparticles by an impurity potential $V$. In the framework of the full Born approximation, QPI for a point-like impurity is proportional to the variation of the LDOS and obtained by \[84, 85\]

$$QPI = \delta N(q||, \omega) = -\frac{V}{\pi} \text{Im}[\Lambda(q||, i\omega)]|_{\omega\rightarrow \omega+i0}. \quad (7)$$

Using the $T$-matrix formalism for a slab geometry \[80\], the QPI function $\Lambda(q||, i\omega)$ is given by

$$\Lambda(q||, i\omega) = \frac{1}{N} \sum_{k_i} \text{Tr}\{\hat{\rho}_0 \hat{G}(k||, i\omega) \hat{G}(k|| - q||, i\omega)\}. \quad (8)$$

Here, the interaction matrix $\hat{\rho}_i = \tau_0 \sigma_i$ acts on the orbital and spin space and distinguishes charge and spin channels, $N$ is the number of grid points. In Fig. 5 we present the QPI at different energies. From (8) one can see that major contributions to the sum are given when both Greens functions have poles simultaneously at $k||$ and $k|| - q||$, i.e. $E_1(k||) \approx E_2(k|| - q||) \approx \omega$. Fig. 5 should therefore be compared to the corresponding momentum-resolved spectral function in Fig. 4(d) at the given $\omega$. As mentioned above, the non-vanishing LDOS at Fermi level is due to the surface states, while the bulk contribution vanishes. As a consequence, the QPI is dominated by the surface states as well at those energies.

We observe that the QPI patterns exhibit divergences when $q||$ connects the surface states at the given $\omega$ on opposite sites of the ring, as shown in the case $\omega = -0.5$. The sharply defined dispersion of the surface states also results in a sign change at the divergence, while the bulk state contribution is smooth, since they form a continuum, e.g. at $\omega = 0.5$ where no surface states are present. Note that the radius of the QPI pattern is twice the radius of the ring at a given energy. As we approach $\omega = 0$ from below, the divergences appear at larger $|q||$ up to twice the radius of the nodal line. At the same time, the surface states become less localized and merge with the bulk states eventually, such that no clear signature from the surface states can be seen at $\omega = 0$.

While the surface state dispersion and therefore the precise form of the QPI patterns depend on the band dispersion of the material, the overall features should be stable under deformations. Especially the sharp divergence and the sign change is a telltale signature of the drumhead surface state, which can be used in STM-based QPI experiments as a fingerprint of the topological surface state.

**B. Weyl nodal line semimetal with antisymmetric SOC**

Let us now discuss how the lack of inversion symmetry affects the topology of a nodal line semimetal. Due to breaking of spatial inversion symmetry through the additional atoms in the unit cell, space group of the candidate materials considered here is $D_{3h}$ (189). This allows for the spin degeneracy to be lifted, resulting in a horizontal shift in the $k$ space in opposite directions for bands of opposite spin upon inclusion of SOC. As a consequence, nodal-line systems without inversion symmetry exhibit Weyl nodal rings with only two-fold degeneracy, which are protected by reflection symmetry along the $z$-direction. Lack of inversion symmetry induces an antisymmetric Rashba or Dresselhaus SOC. The real space Hamiltonian of the WNLS with Rashba and Dresselhaus SOCs is given by

$$\mathcal{H} = \mathcal{H}_0 + \frac{i\alpha}{2} \sum_{(ij), \gamma\gamma', \sigma\sigma'} \hat{\gamma}_{\gamma\gamma'}^z (\hat{\sigma} \times \hat{r}_{ij})_{\sigma\sigma'} c_{i,\gamma,\sigma}^{\dagger} c_{j,\gamma',\sigma'} + \frac{i\beta}{2} \sum_{(ij), \gamma\gamma', \sigma\sigma'} \hat{\gamma}_{\gamma\gamma'}^z (\hat{\sigma} \cdot \hat{r}_{ij})_{\sigma\sigma'} c_{i,\gamma,\sigma}^{\dagger} c_{j,\gamma',\sigma'} \quad (9)$$

where $\alpha$ and $\beta$ are the strengths of Rashba and Dresselhaus SOC. Furthermore, $\sigma$ and $\sigma'$ are spin indices and $\hat{\sigma} = (\hat{\sigma}_z, -\hat{\sigma}_y)$. In momentum space, the Hamiltonian is

![FIG. 6. Energy dispersion of left: $x$, and right: $y$-components of the spin-resolved “surface density of states” along high-symmetry lines of the BZ for (a,d) the Weyl nodal line semimetal (WNLS) with pure Rashba SOC, (b,e) the WNLS with pure Dresselhaus SOC, and (c,f) the WNLS with mixed Rashba and Dresselhaus SOC.](image_url)
given by
\[ H = H_0 + \alpha \sum_{k, \gamma, \sigma, \sigma'} \hat{\tau}^\gamma_{\sigma} (g_k^R \cdot \hat{\sigma})_{\sigma\sigma'} c_{k, \gamma, \sigma} ^\dagger c_{k, \gamma', \sigma'} + \beta \sum_{k, \gamma, \sigma, \sigma'} \hat{\tau}^\gamma_{\sigma} (g_k^D \cdot \hat{\sigma})_{\sigma\sigma'} c_{k, \gamma, \sigma} ^\dagger c_{k, \gamma', \sigma'}, \]
(10)

where \( g_k^R \) and \( g_k^D \) are Rashba and Dresselhaus spin-orbit \( \mathbf{g} \)-vectors and are defined as
\[ g_k^R = \sqrt{3} a \sin\left(\frac{3k_y a}{2}\right) \left[ \cos\left(\frac{3k_x a}{2}\right) + 2 \cos\left(\frac{\sqrt{3}k_y a}{2}\right) \right] \hat{x} - 3a \sin\left(\frac{3k_x a}{2}\right) \cos\left(\frac{\sqrt{3}k_y a}{2}\right) \hat{y}, \]
and
\[ g_k^D = 3a \sin\left(\frac{3k_x a}{2}\right) \cos\left(\frac{\sqrt{3}k_y a}{2}\right) \hat{x} - \sqrt{3} a \sin\left(\frac{\sqrt{3}k_y a}{2}\right) \left[ \cos\left(\frac{3k_x a}{2}\right) + 2 \cos\left(\frac{3k_y a}{2}\right) \right] \hat{y}. \]

Under the operation of parity (\( k \rightarrow -k \)) both spin-orbit \( \mathbf{g} \)-vectors are antisymmetric, i.e., \( g_{-k}^{R/D} = -g_k^{R/D} \). Moreover, Eq. (10) shows that Rashba and Dresselhaus SOCs play the role of momentum-dependent Zeeman fields, thereby splitting the spin degeneracy. Since SOC in this form mixes only states of equal \( R_z \) eigenvalues, the line node is still protected by reflection symmetry.

The energy dispersions of the bulk Hamiltonian (10) at \( k_z = 0 \) along the \( \Gamma \text{K} \text{M} \text{K} \)-path in the presence of a pure Rashba SOC, pure Dresselhaus SOC, and an equal combination of both Rashba and Dresselhaus SOCs are shown in Figs. 2(b) and Figs. 2(c). Due to the presence of antisymmetric SOC, the bulk bands are now spin split. This splitting can be observed in Fig. 4(b), where two separate and concentric Weyl nodal rings are present. Our calculations yield identical results for the case of pure Rashba SOC and pure Dresselhaus SOC. However, mixing of Rashba and Dresselhaus SOC leads to an anisotropic nodal structure in the BZ. We show this in Fig. 4(c) for \( \alpha = \beta \) (i.e., equal strengths of Rashba and Dresselhaus SOCs), in which case the two nodal rings intersect each other along the [11] direction. This anisotropy can also be seen in the asymmetry of the dispersion in \( K \rightarrow \Gamma \) and \( \Gamma \rightarrow M \) directions in Fig. 2(c).

With the same approach as for the case of DNLs, we investigate the surface states and the topological properties of WNLS using an \( xy \)-slab geometry. However, for WNLSs, we now need to take the spin degrees of freedom into account. The slab Hamiltonian for the WNLSs is of the same form as Ref. [3], with the following spin-dependent hopping matrices
\[ M = [\hat{\varepsilon}_1 k_{\|} - t' \hat{\tau}_z] \hat{\sigma}_0 + [\alpha g_y^R(k_{\|}) + \beta g_y^D(k_{\|})] \hat{\tau}_z \hat{\sigma}_x + [\alpha g_y^R(k_{\|}) + \beta g_y^D(k_{\|})] \hat{\tau}_z \hat{\sigma}_y, \]
\[ T = - \left[ t_\perp \hat{\tau}_z + \frac{1}{2} t' \left( \hat{\tau}_x - i \hat{\tau}_y \right) \right] \hat{\sigma}_0, \]
(11)

where \( \hat{\sigma}_i \) operates in spin space and \( g_y^{R/D} \) and \( g_y^{R/D} \) are \( x \)- and \( y \)-components of the Rashba/Dresselhaus \( \mathbf{g} \)-vectors. Figs. 2(e) and 2(f) portray the momentum-resolved spectral functions for the surface slab of the WNLS with pure Rashba/Dresselhaus and their combination with equal strengths. The horizontal shifts in the band structures due to SOC is clearly observed. In addition, one can see that in the presence of both Rashba and Dresselhaus SOC, the topological surface states become anisotropic. In Figs. 4(e) and 4(f) we present the momentum-resolved spectral functions at zero energy, \( \omega = 0 \), for the surface slab of the WNLSs. Figure 4(e) corresponds to a WNLS with pure Rashba/Dresselhaus SOC. Here, two isotropic and concentric drumhead surface states are observed. In Fig. 4(f), one can see two shifted drumhead surface states of equal width, which stem from an interplay between Rashba and Dresselhaus SOC with equal strengths.

C. Spin texture of Weyl nodal line semimetals

Antisymmetric SOC splits the spin degeneracy of the bands, thereby creating a nontrivial spin texture of the bulk and surface band structure of WNLSs. Therefore, compared to a DLNS, the band structure in a WNLS is strongly spin polarized. Due to the locking of orbital and spin degrees of freedom by SOC, none of the spin and momentum can be supposed as well-defined quantum numbers. Consequently the Hamiltonian doesn’t remain diagonal in spin space. For diagonalizing the Hamiltonian of a WNLS, one has to change the basis to the helicity basis (\( |\pm\rangle \)). In the helicity basis, the expectation values of the different components of the spin operator, \( \hat{S}^i \), are given by
\[ \langle \hat{S}^i \rangle_\pm = \langle \pm | \hat{S}^i | \pm \rangle = \pm g^i_k, \]
(12)
with \( g^i_k = g^i_k / |g_k| \). Along the \( \Gamma \rightarrow M \) path the momentum component \( k_y \) is zero, \( k_y = 0 \), and consequently Eq. (12) implies that \( g^x_k \) and \( g^y_k \) are zero in a WNLS with pure Rashba and pure Dresselhaus SOC, respectively. Therefore the \( x \)-component (\( y \)-component) of the spin polarization of the WNLS with pure Rashba (pure Dresselhaus) SOC is zero in the above-mentioned direction.

In the same way as in the bulk, the spin degeneracy of the surface states of the WNLS is lifted and they become spin polarized. To examine the spin texture of the
topological surface states, we are using the spin-resolved spectral function. For the nth slab it is defined as

$$\rho_{\alpha}^{n}(k_{||}, \omega) = -2\text{Im} \left\{ \text{Tr} \left[ \hat{S}^{i} \hat{G}^{ret}_{nn}(k_{||}, \omega) \right] \right\}, \quad (13)$$

where $\hat{S}^{i} = \tau_{0} \frac{1}{2} \sigma^{i}$. As seen in Figs. 4(g)-4(i), antisymmetric Rashba and Dresselhaus SOC generate two concentric spin-polarized drumhead surface states, whose total spin polarizations are inside the $xy$-plane. One can clearly observe that the Weyl nodal rings are fully spin-polarized in opposite directions. Figures 6(a-f) show the $x$- and $y$-components of the spin-resolved spectral functions along the KFMK-path for the first slab of a WNLS with (a,d) pure Rashba SOC, (b,e) pure Dresselhaus SOC, and (c,f) mixed Rashba and Dresselhaus SOC.

In order to investigate the effect of SOC via QPI, we have to move from non-magnetic to magnetic impurities. Scattering at non-magnetic impurities allows for scattering between states of the same spin orientation. From the spin polarization of the surface states it becomes clear, that the contribution from the surface states is given by inter-surface state scattering only. Therefore, the shift in the radius of the two nodal lines is not visible and the pattern looks almost identical to the spinless case.

For a magnetic impurity in $z$-direction, which can be controlled by applying a small magnetic field, the scattering involves a spin flip for all states, since they are all in the $xy$-plane. For this case, Eq. (8) in the calculation of the QPI pattern contains the spin matrix of the impurity and is modified to

$$A^{(3,3)}(q_{||}, i\omega) = \frac{1}{N} \sum_{k_{||}} \text{Tr} \left[ \hat{\theta}_{3} \hat{G}(k_{||}, i\omega) \tau_{0} \sigma_{3} \hat{G}(k_{||} - q_{||}, i\omega) \right]. \quad (14)$$

The spin resolved QPI in $z$-direction for such an impurity is sensitive to the intra-band scattering only, while all inter-band contributions are suppressed now. We present the patterns for the above mentioned cases in Fig. 7. Each of the surface states contributes their own divergence when $q$ equals the diameter, leading to the double ring structure.

III. CONCLUSIONS

In this paper, we have studied the topological surface states of Dirac and Weyl nodal-line semimetals, whose nodal lines are protected by reflection and time-reversal symmetry. In the presence of spatial inversion symmetry, our two-orbital tight-binding model corresponds to a Dirac nodal line semimetal with a four-fold degenerate band crossing, supporting the realization of spin degenerate drumhead surface states. In the absence of inversion symmetry, by including antisymmetric Rashba and Dresselhaus SOC, our model describes a topological Weyl semimetal with two-fold degenerate nodal rings. We have shown that pure Rashba and pure Dresselhaus SOC have the same effects on the topology of the electronic band structure and the surface states. In addition, we have found that in the presence of mixed Rashba and Dresselhaus SOC, the Weyl nodal rings become anisotropic. Since antisymmetric SOC lifts the spin degeneracy, the drumhead surface states of Weyl nodal line semimetals are strongly spin-polarized with a spin polarization vector within the $xy$-plane. By evaluating the Berry phase, we have demonstrated that the drumhead surface states of the Dirac and Weyl nodal-line semimetals arise from the non-trivial topology of the band crossing in the bulk.

We have also computed the quasiparticle interference (QPI) patterns for the surface of Dirac and Weyl nodal-line semimetals and have shown that these interference patterns contain unique signatures of the drumhead surface states. Namely, for the Dirac nodal-line semimetal there appears a single ring, both in the ordinary and in the spin-resolved QPI patterns (Fig. 5). However, for the Weyl nodal-line semimetal there appear two rings in the spin-resolved QPI pattern, see Fig. 7. We have checked that these features do not depend on the particular parameter choice. They are therefore generic to any nodal-line material and should be observable in Fourier-transform scanning tunnelling spectroscopy. The wavelength of the Friedel oscillations, giving rise to the ring in the QPI pattern, depends on the size of the Dirac or Weyl nodal ring in the bulk. For example, in CaAgAs the nodal ring has a radius of about $0.1 \ \text{Å}^{-1}$ [42], while in PbTaSe$_2$ it is about $0.2 \ \text{Å}^{-1}$ [6]. Hence, the Friedel oscillations have a wavelength of about $10 - 30 \ \text{Å}$, which should be measurable in STM experiments. With regards to energy resolution, we find that the gap within which the drumhead state exists, is typically of the order of a few 100 meV and the SOC is typically about 50-100 meV [6, 7, 42]. These energy scales are easily resolvable with STM. We hope that our findings will stimulate such experiments.
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appendix a: theory of qpi for a semimetal

here we develop the theory of qpi for a dirac or weyl nodal line semimetal in the presence of particle-hole symmetry. we employ the matsubara green’s function in a generalized orbital and spin space, which is described by the field operator \( \psi_k \). the general orbital and spin space, which is described by the field operator \( \psi_k \). the green’s function on this space is given by

\[
\hat{G}(k, i\omega) = \begin{bmatrix}
\hat{G}^+(k, i\omega) & \hat{F}(k, i\omega) \\
\hat{F}^+(k, i\omega) & \hat{G}^-(k, i\omega)
\end{bmatrix},
\]

where in a \( 2 \times 2 \) spin space representation, \( \hat{G}^\pm(k, i\omega) \) and \( \hat{F}(k, i\omega) \) are matsubara green’s functions for intra- and inter-orbital hopping, respectively. in the presence of spin-orbit coupling, the bare green’s functions are expressed as

\[
\hat{G}^\pm(k, i\omega) = \frac{1}{2} \sum_{\xi, \xi'} (\sigma_0 + \xi \hat{g}_k \cdot \sigma) \hat{G}_\xi^\pm(k, i\omega),
\]

\[
\hat{F}(k, i\omega) = \frac{1}{2} \sum_{\xi, \xi'} \hat{F}_\xi(k, i\omega) \sigma_0,
\]

where \( \hat{g}_k = \hat{g}_k/|\hat{g}_k| \) with

\[
\hat{G}_\xi^\pm(k, i\omega) = \frac{i\omega \pm \varepsilon_1(k) \pm \xi |\hat{g}_k|}{(i\omega)^2 - E_{k\xi}^2},
\]

\[
\hat{F}_\xi(k, i\omega) = -i\varepsilon_2(k)/((i\omega)^2 - E_{k\xi}^2),
\]

in which

\[
E_{k\xi} = \sqrt{(\varepsilon_1(k) + \xi |g|)^2 + \varepsilon_2^2(k)}
\]

is the energy dispersion with helicity \( \xi \). the modulation of ldos is calculated by taking the effect of scattering from magnetic or nonmagnetic impurities into account. the impurity hamiltonian has the form

\[
\hat{H}_{imp} = \sum_{kq\delta} V(q) \psi_{k+q}^\dagger \hat{\delta} \psi_k,
\]

where \( \{ \hat{\delta} \} = \tau_0 \sigma_\delta \) is the spin of the impurity site. the case \( \delta = 0 \) corresponds to scattering from a nonmagnetic impurities and the cases \( \delta = x, y, z \) are related to scattering via magnetic impurities. the changes in the stm tunneling conductance due to impurity scattering can be evaluated by

\[
\frac{d(\Delta I_\delta)}{dV} \sim \Delta N_{\delta\delta'}(r, \omega = V) = -\frac{1}{\pi} \text{Im} \left[ \text{Tr}_\sigma \hat{\delta} \hat{\delta} \Delta \hat{G}_{\delta'}(r, r, \omega) \right],
\]

where, \( \Delta \hat{G}_{\delta'} \) is the change of \( 4 \times 4 \) matrix of green’s function due to impurity scattering from a charges (\( \delta' = 0 \)) or magnetic (\( \delta' = x, y, z \)) impurity.

it is common to define qpi as the fourier transformed modulation of the ldos from the scattering at an impurity,

\[
\Delta N_{\delta\delta'}(q, \omega) = -\frac{1}{\pi} \sum_r e^{iq \cdot r} \text{Tr}_\sigma \frac{1}{2i} \left[ \hat{\delta} \Delta \hat{G}_{\delta'}(r, r, \omega) - (\hat{\delta} \Delta \hat{G}_{\delta'}(r, r, \omega))^* \right]_{\omega \rightarrow \omega + i0^+}.
\]
where
\[
\Lambda_{\delta\delta'}(q, \omega) = \frac{1}{N} \sum_k \text{Tr}_\sigma \left[ \hat{G}_0(k, \omega) \hat{G}_0(k - q, \omega) \right],
\]
and \(N\) is the number of grid points and \(\hat{G}_0\) is the Greens function of the unperturbed system. When \(\Lambda_{\delta\delta'}\) is symmetric in \(q\), the bracket in Eq. (A8) reduces to \(\text{Im} \Lambda_{\delta\delta'}(q, \omega)\). Finally, the QPI function \(\Lambda_{\delta\delta'}\) is obtained as [84, 85]
\[
\begin{align*}
\Lambda_{00}(q, \omega) &= \frac{1}{4N} \sum_{k\xi'\xi} \left[ \left(1 + \xi\xi'(\hat{g}_k \cdot \hat{g}_{k-q}) \right) K^{kq}_{\xi\xi'}(\omega) + K^{kq}_{\xi'\xi}(\omega) \right]; \\
\Lambda_{ii}(q, \omega) &= \frac{1}{4N} \sum_{k\xi'\xi} \left[ \left(1 - \xi\xi'(\hat{g}_k \cdot \hat{g}_{k-q} - 2\hat{g}_k^i \hat{g}_{k-q}^i) \right) K^{kq}_{\xi\xi'}(\omega) + K^{kq}_{\xi'\xi}(\omega) \right],
\end{align*}
\]
with the integration kernels
\[
K^{kq}_{\xi\xi'}(\omega) = \frac{[\omega + \epsilon_1(k) + \xi(\hat{g}_k \cdot \hat{g}_{k-q})]}{[\omega - \epsilon_k^2]}; \\
P^{kq}_{\xi\xi'}(\omega) = \frac{\epsilon_2(k)\epsilon_2(k - q)}{[\omega - \epsilon_k^2]};
\]
\[\Lambda_{\delta\delta'}(q, \omega) = \frac{1}{N} \sum_k \text{Tr}_\sigma \left[ \hat{G}_0(k, \omega) \hat{G}_0(k - q, \omega) \right],\]

\[\text{APPENDIX B: BERRY PHASE}\]

The Berry phase is obtained through the eigenvalues of the Wilson loop matrix for a closed path enclosing the nodal ring. For a closed loop, the Berry phase \(\mathcal{P}\) is given by
\[
\mathcal{P}(k_x, k_y) = i \ln \left| \text{det}(W_L(k_x, k_y)) \right|, \quad (B1)
\]
where the discrete Wilson loop matrix is given by the product of the link matrices, \(U_n\), made up by the occupied bands \(|u_n(k_n)\rangle\) at each step \(k_n \rightarrow k_{n+1}\) along the closed path \(k_0 \rightarrow k_N = k_0 + G\), with \(G\) as the lattice translation vector of the reciprocal lattice,
\[
W_L = \prod_{n=0}^{N-1} U_n / \left| \text{det}(U_n) \right|, \quad (B2)
\]
by the link matrix’s elements defined as
\[
U_n^{ij} = \langle u_i(k_n) | u_j(k_{n+1}) \rangle . \quad (B3)
\]
Whenever the Berry phase \(\mathcal{P}(k_x, k_y) \neq 0\), a nontrivial in-gap state appears for \((k_x, k_y)\) at the surface BZ. The non-trivial Berry phase for band crossing around \(\Gamma\) in BZ guarantees the stability of topological drumhead surface states [See Fig. 3(a)].
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