Infinite Berry curvature of Weyl Fermi arcs

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We show that Weyl Fermi arcs are generically accompanied by a divergence of the surface Berry curvature scaling as \(1/k^2\), where \(k\) is the distance to a hot-line in the surface Brillouin zone that connects the projection of Weyl nodes with opposite chirality but which is distinct from the Fermi arc itself. Such surface Berry curvature appears whenever the bulk Weyl dispersion has a velocity tilt toward the surface of interest. This divergence is reflected in a variety of Berry curvature mediated effects that are readily accessible experimentally, and in particular leads to a surface Berry curvature dipole that grows linearly with the thickness of a slab of a Weyl semimetal material in the limit of long lifetime of surface states. This implies the emergence of a gigantic contribution to the non-linear Hall effect in such devices.

Introduction. The Berry curvature (BC) of electronic bands is known to deeply influence a variety of properties and phenomena [1]. Therefore, one of central quests of modern material design is to find mechanisms that can lead to large enhancements of BC. Typically large BC concentrations occur at points in Brillouin zone (BZ) where two bands are exactly or nearly degenerate, leading to rapid changes of the Bloch wavefunctions near such hot-spots. Classic examples of such BC hot-spots include the Weyl nodes in 3D materials [2, 3] and the Dirac points in 2D graphene. In this letter, we will demonstrate a distinct mechanism by which a divergence of BC occurs not at a point, but instead over an entire line in the BZ, which we will refer to as a “hot-line”. These hot-lines emerge in the surface BZ of Weyl semimetals [2, 3] (WSMs), and they separate the 2D states that are localized at the surface from the continuum of 3D bulk states. Therefore, whereas the hot-line is distinct from the surface Fermi arc, they will meet at the momentum where the Fermi arc terminates and mixes with 3D bulk states, as illustrated in Fig. 1. The BC divergence at these hot-lines will be generically present in the WSM surface states whenever a bulk Weyl node has a velocity-tilt with a component normal to the surface of interest.

This large enhancement of BC at a hot-line is expected to manifest in a variety of contributions to physical effects in WSMs. In particular, we will demonstrate that it can lead to gigantic contribution to the BC driven non-linear Hall effect [4–16], featuring a contribution to the Berry-curvature-dipole (BCD), \(D\), that grows linearly proportionally with the thickness, \(L\), of a WSM slab:

\[ D \propto L \]  

This contribution can arise even when there is no bulk Fermi surface (chemical potential is at the bulk Weyl node), so that there is nominally no 3D bulk BCD. Our findings not only enhance the understanding of the geometrical aspects of the Fermi-arcs electronic structure but also should be experimentally relevant in all BC driven phenomena in Weyl semimetals.

We will illustrate this phenomena first in an ideal model containing a single Weyl node in a semi-infinite geometry which allows a simple conceptual understanding. We will then progressively extend this model to include the fact that Weyl nodes always come in pairs [17] and the effects of finite thickness \(L\). We will then provide quantitative estimates for WSMs TaAs and TaP based on first principles calculations.
**Single Weyl node model.** We consider a low energy model of a single Weyl cone \((\hbar = 1)\)
\[
H = -i\nabla \cdot (\chi \mathbf{v}_F \sigma + \mathbf{u} \sigma_0),
\]  
with chirality \(\chi = \pm 1\), Fermi velocity \(v_F > 0\), and tilt velocity \(\mathbf{u}\). Here \(\sigma\) is the vector of Pauli matrices and \(\sigma_0\) is the identity. In the following we set \(v_F = 1\) and without loss of generality we assume that the surface normal \(\mathbf{n}\) of a semi-infinite WSM residing at \(z < 0\) points into the \(z\)-direction, \(\mathbf{n} = \hat{z}\). The wave function is therefore viewed as having non-zero amplitude only for \(z \leq 0\). As discussed in Refs. [18–22], in order to guarantee hermiticity of the Hamiltonian from Eq. (15), the following boundary condition of vanishing current density normal to the surface must be imposed:
\[
\psi^\dagger \sigma_z \psi|_{z=0} = -\chi u_z \psi^\dagger \psi|_{z=0}.
\]
Therefore, remarkably, the normal component of the pseudo-spin density at the boundary is determined by the normal component of the tilt velocity, leaving its component parallel to the boundary as a free parameter. We therefore parametrize the orientation of the pseudo-spin density at the boundary by a unit vector \(\mathbf{s}\):
\[
\mathbf{s} = \left(\sqrt{1-u_z^2} \cos(\alpha), \sqrt{1-u_z^2} \sin(\alpha), -\chi u_z \right).
\]
Within our continuum model of semi-infinite space, \(\alpha\) is an undetermined parameter. However, \(\alpha\) is understood to be uniquely fixed in an underlying microscopic description. One way to do this is to solve a continuum model in the entire space that includes an explicit description of the decay of the wave-function into vacuum, as we illustrate in the Suppl. Materials [23] in Sec. B. Moreover, although \(\alpha\) is unique in any microscopic Hamiltonian defined for all \(z\), it can depend on microscopic details of the boundary [20] and on band-bending effects [18]. In writing Eq. (17) we are assuming that the system is a type-I WSM [23] with |\(\mathbf{u}\)| < \(v_F\).

Wave functions localized at the boundary have the form \(\Psi(\mathbf{k}_||, z) = e^{ik||x + k||y} r_|| \psi\) with Re\(\lambda\) > 0, and \(r_||\), \(k||\) denoting the coordinates and momentum parallel to the boundary. Their dispersion is found to be (see Suppl. Materials [23], Sec. A)
\[
E_{k||} = k|| \cdot (\chi \mathbf{s} + \mathbf{u}),
\]
and
\[
\lambda = -\frac{k|| \cdot (\mathbf{n} \times \mathbf{s} + i\chi u_z \mathbf{s})}{1 - u_z^2}.
\]
The Fermi arc at \(E_{k||} = 0\) is therefore a straight ray pointing in the direction \(\mathbf{n} \times (\chi \mathbf{s} + \mathbf{u})\) and starting from the projection of the Weyl node onto the surface of interest as illustrated in Fig. 1(a). The surface BC is given by \(\Omega_z = \partial k_x A_y - \partial k_y A_x\) with Berry connection
\[
\mathbf{A}(\mathbf{k}_||) = -i \int_{-\infty}^{0} dz \psi^\dagger (\mathbf{k}_||, z) \nabla_{k||} \psi(\mathbf{k}_||, z),
\]
which yields:
\[
\Omega_0(\mathbf{k}_||) = -\frac{\chi u_z (1 - u_z^2)}{2 (k|| \cdot (\mathbf{n} \times \mathbf{s}))^2} \mathbf{n},
\]
where \(|\mathbf{n} \times \mathbf{s}|^2 = 1 - u_z^2\) and is fully determined by the tilt \(\mathbf{u}\), the surface normal \(\mathbf{n}\), chirality \(\chi\), and boundary spin polarization direction \(\mathbf{s}\). The equation above summarizes one of our central findings: The BC of the surface diverges quadratically as the surface momentum approaches the hot-line defined by \(k|| \cdot (\mathbf{n} \times \mathbf{s}) = 0\) which separates the states localized at the surface, that have \(\text{Re}(\lambda) > 0\) in Eq. (21), from those that mix with the 3D bulk (see Fig. 1(a)). We emphasize that this divergence occurs over an entire line in the surface momentum plane (the surface BZ in a lattice model) and not just on the single point. Notice also that this hot-line is distinct from the Fermi arc, but the Fermi arc always terminates at a point in this line independent of the Fermi energy. Furthermore, the BC is proportional to \(u_z\) and vanishes if the Weyl cone is not tilted toward the surface. Since \(u_z = \mathbf{u} \cdot \mathbf{n}\) the surface state has the same BC on the top and bottom surface with \(\mathbf{n} \rightarrow -\mathbf{n}\). Divergences of the BC typically encode a rapid change of the intra-unit cell Bloch wavefunction as a function of the crystal momentum. Although the commonly known BC hot-spots around a bulk Weyl node originate from the rapid change of the wavefunction pseudospin as the node is crossed staying within the lower branch, the divergence of BC at the surface hot-line originates from a different underlying mechanism. The BC hot-line does not originate from a rapid change of the pseudo-spin, whose orientation remains essentially constant upon approaching the line, but rather from an abrupt change of the localization of the wavefunction along the direction orthogonal to the surface. This is why it coincides with the line that separates bulk from surface-localized states. In experiments this BC can be probed via the Berry curvature dipole \(\mathbf{D} = \frac{1}{2} \int d^2\mathbf{k}_|| \frac{\Omega_0}{(2\pi)^2} \mathbf{n} \nabla_{k||} n_f\)
where \(n_f\) is the Fermi-Dirac distribution. Since the BC diverges at the end of the Fermi arc, the Fermi arc contribution to BCD also diverges. It is instructive to consider the regularization of this divergence by introducing a cutoff at distance \(k_c\) from the hot-line in momentum space. We will discuss how to obtain \(k_c\) later in a finite slab geometry. For a single Weyl cone we then find the following Fermi arc contribution to the surface BCD at zero temperature
\[
\mathbf{D} = -\frac{\chi u_z}{8\pi^2 k_c} \sqrt{1 - u_z^2} \frac{\mathbf{s} + \chi \mathbf{u}}{1 + \chi \mathbf{s} \cdot \mathbf{u}},
\]
which thus scales as $D \propto u_\perp/k_\perp$ and is perpendicular to the Fermi arc as depicted in Fig. 1 (a). Although we have taken zero temperature, one can verify that the Fermi arc contribution to the BCD remains infinite at finite temperature and it is independent of the chemical potential.

Weyl pair model. Fermi arcs on crystal surfaces always connect projections of two Weyl nodes with opposite chirality. In order to get a low-energy Hamiltonian for a pair of Weyl cones \cite{13 16 22} we modify the Hamiltonian in Eq. \eqref{15} by substituting

$$k_y \to \tilde{k}_y = \frac{k_0^2 - k_y^2}{2k_0}. \quad (11)$$

The two Weyl nodes with chirality $\pm \chi$ are located at $k_y = \mp k_0$ ($k_0 > 0$) and $k_z = k_\perp = 0$ and are related by a mirror symmetry $M_y$. This symmetry acts only in the spatial part but not the pseudospin $\sigma$, and thus it is not broken by the boundary condition in Eq. \eqref{16}. For simplicity, we take here $u = u_\perp n$. Again, if we perform an analogous analysis as in the single Weyl node we are led to boundary conditions parametrized by the vector $s$ from Eq. \eqref{17}. The Fermi arc becomes a parabola between the nodes as illustrated in Fig. 2 (b) where the free parameter $\alpha = \gamma$ is the angle between $k_\perp$-axis and the Fermi arc at the node. The arc connects the Weyl nodes for $|\alpha| < \pi/2$, in a lattice model the nodes would also be connected for larger values of $\alpha$ via the periodic boundaries of the lattice BZ. We have verified that an alternative model with an explicit interface between vacuum and the WSM recovers the results of this model for the special case of $\alpha = 0$ (see SM \cite{24}, Sec. B).

In this semi-infinite system the surface BC is again diverging at the ends of the Fermi arc and the hot-line becomes a parabola, and it is given by

$$\Omega (k_\parallel) = - \frac{\chi u_\perp k_y}{2k_0 \left( k_x \sin(\alpha) - \tilde{k}_y \cos(\alpha) \right)^2}. \quad (12)$$

Notice that as a consequence of the $M_y$ mirror symmetry the BC changes sign at $k_y = 0$ and the BCD only has non-zero $D_y$ component. Since most of the BC of the Fermi arc is located close to the nodes, the size of the BCD of a Weyl pair is approximately twice the $D_y$ component of the BCD of a single node.

Weyl nodes in finite slabs. As we have discussed there is a remarkable divergence of the surface BC and the surface BCD of ideal Fermi arcs in semi-infinite geometries. In real materials a variety of physical effects can regularize such divergence such as the finite lifetime of surface states induced by disorder or phonons. Here we will focus on the limit in which the lifetime associated with the decay of surface quasiparticles into the bulk is much longer than the intra-surface scattering time. In this limit the regularization of these effects arises from the finite thickness of the material. To do so we restrict the WSM to reside within $|z| \leq L/2$. As detailed in the SM \cite{24}, Sec. C, hermiticity now requires $\chi z_\perp - u_z$ to be the same on both surfaces. Nevertheless, the parallel component $s_\parallel$ is again not fixed and can have a different angle on top and bottom surface. We define these two free parameters to be the angle $\pi - 2\gamma$ between the top and bottom spin polarization with $|\gamma| < \pi/2$, and the angle $\theta$ between $s_\parallel$ for $\gamma = 0$ and positive $k_\perp$-axis. Without loss of generality we can set $\theta = 0$, i.e. for $u_\perp = 0$ the Fermi arcs are located around the $k_\perp$-axis with angle $\pm \gamma$ as shown in Fig. 3 (b).

The energy dispersion of the surface states can be conveniently parametrized in terms of the function $\epsilon(k_\parallel)$, as

$$E (k_\parallel) = \chi \sqrt{1 - u_\perp^2 \epsilon(k_\parallel) + k_\parallel \cdot u},$$

which in turn is defined implicitly as a solution of the following transcendental equation:

$$\sqrt{k_\parallel^2 - \epsilon^2} = \frac{k_y - \epsilon \sin(\gamma) \tanh \left( \frac{L \sqrt{k_\parallel^2 - \epsilon^2}}{1 - u_\perp^2} \right). \quad (13)$$

The resulting energy dispersion is illustrated in Fig. 2 (a). The decay length of these solutions into the bulk is given by $\text{Re}(\lambda) \propto \sqrt{k_\parallel^2 - (\epsilon(k_\parallel))^2}$. Therefore the surface states of our interest correspond to the two solutions with $(\epsilon(k_\parallel))^2 < k_\parallel^2$. In the $L \to \infty$ limit this equation recovers the energy dispersion from Eq. \eqref{20} for each surface. Fig. 2 shows that for finite $L$ a gap opens at the
intersection of the two orange surface bands, which decreases exponentially in system size and distance from the Weyl node. This opening of a gap gives rise to the fact that neither the Fermi arc nor the hot-line touches the Weyl point anymore but hybridizes with the arc/line from the opposite surface for finite $L$. The Fermi arc and the hot line will, however, touch the surface projection of the Weyl node for $L \rightarrow \infty$ (see Fig. 1(b) and Fig. 1 in SM [23] for an illustration). A first order Taylor expansion of Eq. 13 around $c^2 = k^2_z$ determines the BC hot-line depicted as a solid black line in Figs. 1(b) and 2 where the surface state becomes a bulk state. The minimal distance of the BC hot-line to the Weyl node is given at $k_x = 0$ and $k_y = k_c$ with
\[ k_c = \frac{\sqrt{1 - u_z^2}}{L \cos(\gamma)} (1 - \sin(\gamma)), \] (14)
which serves as a momentum cutoff for the BCD, as discussed in the previous section.

This leads to the remarkable conclusion that, ideally, the Fermi arc contribution to the BCD increases with the thickness $L$ of the crystal slab. Therefore, since our model of a single Weyl node contains as its only length scale the slab thickness $L$, and the BCD has units of length in 2D [6], this model predicts a BCD that is exactly linearly proportional to $L$, without the need of any explicit cutoff. Additionally, Fig. 2(b) shows the direct numerical calculation of the BC for our model of a pair of Weyl nodes from Eq. 11 in a finite slab geometry. As we see there are some notable modifications brought in by the pair of Weyl cones in a finite size. In particular the BC is highly peaked around $k_x = 0$, i.e. where the surface state changes from top to bottom surface.

**Experimental signatures.** WSMs exist only in materials breaking either spatial inversion or time-reversal (TR) symmetry. Our results can be applied generally to materials that break either of these symmetries by considering additional symmetry related copies of the elementary models of Weyl cones that we have studied, and thus Weyl Fermi arcs generically display the infinite Berry curvature at hot-lines that we have described. In the special case in which the material is time reversal invariant and the non-linear Hall effect is the leading Hall-like response, the surface BCD will remain non-zero after adding symmetry related copies of the models. More precisely, two Weyl node pairs that are related by TR will have additive contributions to the BCD.

Candidate materials for observing the giant non-linear Hall effect resulting from this Fermi arc contribution to the BCD include, in principle, all 3D type-I WSMs with broken inversion symmetry. For example, WSMs TaAs and TaP [14] are TR symmetric and well suited for experiments. We performed density-functional (DFT) calculations for these two compounds using a generalized gradient approximation [25] as implemented in the FPLO code [26]. As in previous reports [27, 28], we find a set of four pairs of Weyl nodes in the $k_z = 0$ plane and a second set of eight Weyl nodes away from such plane. In the following, we will focus in the latter set, named $W_2$, which is of type I in TaAs and TaP, and placed closer to the Fermi energy. Detailed values for the fit of the DFT data to our model can be found in the SM [23] in Sec. D. WSMs of the TaAs family belong to the point group $C_{4v}$, i.e. these materials have a polar axis in $z$-direction allowing a bulk BCD [13] [14] [16].

In order to have a non-vanishing net BCD, the maximal symmetry of the finite system including its surfaces should be a mirror line [6]. Such mirror line forces the direction of the BCD to be perpendicular to it. Furthermore, symmetries such as bulk mirror planes parallel to the surface must be avoided since they project Weyl nodes of opposite chirality onto the same point in the surface Brillouin zone. It is interesting, in particular, to consider materials that are nominally inversion invariant in the bulk, but the 3D inversion of the slab is broken by a surface effect, such as the asymmetry between top and bottom surfaces that one would have when the slab resides in a substrate. In these cases, the non-linear Hall effect will be dominated by the surface states allowing one to directly probe the divergence of the surface Berry curvature of the Weyl Fermi arcs. For WSMs of the TaAs family the crystal symmetries allow all cones to be tilted perpendicular to the 4-fold rotation axis. Due to this rotation axis the (001) surface does not exhibit a surface BCD, as well as a surface parallel to one of the mirrors belonging to this axis. Nevertheless, a suitable surface which keeps a single mirror line $M_x$ and has proper tilted cones is, for instance, (011). Depending on $\alpha$, the BCD of a single $W_2$, Weyl pair can reach up to $D_x = 0.042L$ in TaAs and $D_x = 0.041L$ in TaP on this surface.

The BC divergence at the hot-line should have interesting consequences in many phenomena [1]. In addition to the non-linear transport signatures, the BCD $D$ also induces an effective orbital magnetization $M \propto D \cdot E_{z}$ in the presence of an electric field $E$ which can be measured using Kerr rotation or circular dichroism [29]. A further experimental probe is the second order response to an applied thermal gradient $\nabla T$ [30]. The nonlinear anomalous Nernst effect is a current perpendicular to the temperature gradient and proportional to $(\nabla T)^2$, which at low temperatures is linear in the BCD [31]. Other interesting potential manifestations of this divergence could appear in the surface contributions to the orbital magnetic moment of materials with bulk Weyl nodes [32, 33], and also in the surface contributions in the non-linear version of the chiral anomaly [35].

**Concluding remarks.** We have demonstrated the existence of a generic divergence of the Berry curvature at a hot-line in the surface of Weyl semimetals, which is distinct from the Fermi arc itself. This divergence scales as the inverse square distance in momentum space to
SUPPLEMENTARY INFORMATION

A Surface wave function for semi-infinite system

Here we give the full surface wave function of a semi-infinite Weyl semimetal (WSM) with a tilted cone. We start from the low energy Hamiltonian

\[ H = -i \nabla \cdot (\chi \sigma + u \sigma_0) \]  

and restrict it to \( z \leq 0 \) such that we get a surface with normal \( n = \hat{z} \). This makes it convenient to split every vector in a parallel and perpendicular part, e.g. \( u = u_{\parallel} + u_{\perp} n \) with \( u_{\parallel} \perp n \). The Hamiltonian is translational invariant parallel to the surface which allows us to replace \(-i \nabla \to k_{\parallel} - i m \partial_{z} \). By partial integration one can show that hermiticity \( \langle \psi_1, H \psi_2 \rangle = \langle H \psi_1, \psi_2 \rangle \) of the Hamiltonian requires the boundary term at \( z = 0 \) to vanish [18,22], i.e.

\[ \psi_{1}^\dagger (\chi \sigma_z + u_{z}) \psi_{2}|_{z=0} = 0 \]  

for all \( \psi_1, \psi_2 \). Here we look at the special case where \( \psi_1 = \psi_2 \equiv \psi, |\psi|^2 = 1 \), are \( z \)-independent spinors so that the expectation value \( s \) of the pseudo-spin for \( \psi \equiv \psi(\alpha) \) can be written as

\[ s = \left( \sqrt{1 - u_{z}^2 \cos(\alpha)}, \sqrt{1 - u_{z}^2 \sin(\alpha)}, -\chi u_{z} \right) \]  

with free real parameter \( \alpha \) labeling all possible boundary conditions. For the surface wave function \( \Psi \) we make the ansatz

\[ \Psi \left( k_{\parallel}, z \right) = c \left( k_{\parallel} \right) e^{i k_{\parallel} \cdot r_{\parallel} + \lambda \chi_{\parallel} z} \psi(\alpha) \]  

where \( c(k_{\parallel}) \) is the (real) normalization constant. Since \( \Psi \propto \psi(\alpha) \) for all \( z \) the boundary condition Eq. [16] always is fulfilled. In order to obtain a surface state the function \( \lambda(k_{\parallel}) \) must have a non-vanishing real part.

More precisely, normalization \( 1 = \int_{0}^{\infty} dz \, |\Psi|^2 \) gives \( c^2 = 2 \text{Re}(\lambda) \) and requires \( \text{Re}(\lambda) > 0 \). Applying the gradient of the Hamiltonian in Eq. [15] to wave function \( \Psi \) yields the effective Hamiltonian

\[ H_{\text{eff}} = k_{\parallel} \cdot (\chi \sigma + u_{z} \sigma_0) - i\lambda (\chi \sigma_z + u_{z} \sigma_0) \]  

Note that we are not dealing with non-hermitian Hamiltonians since \( (\chi \sigma_z + u_{z} \sigma_0) \Psi = 0 \) due to the boundary condition. Thus, the energy \( H \Psi = H_{\text{eff}} \Psi = E \Psi \) becomes

\[ E(k_{\parallel}) = k_{\parallel} \cdot (\chi s + u) \]  

The function \( \lambda(k_{\parallel}) \) can be obtained by solving \(-\chi u_{z} E(k_{\parallel}) = \langle \psi | H_{\text{eff}} \sigma_{z} | \psi \rangle \) for \( \lambda \). This yields

\[ \lambda = -\frac{k_{\parallel} \cdot (n \times s + i \chi u_{z} s)}{1 - u_{z}^2} \]  

Finally, from \( \psi^\dagger \sigma \psi = s \) we find

\[ \psi(\alpha) = \frac{1}{\sqrt{2}} \left( e^{-i \alpha/2} \sqrt{1 - \chi u_{z}} \right) \left( e^{i \alpha/2} \sqrt{1 - \chi u_{z}} \right) \]
Figure 3. Fermi arc and hot-line in a finite slab with width \( L = 3 \) (left) and \( L = 10 \) (right). The dashed lines mark the Fermi arc and hot-line for \( L \to \infty \).

**B Explicit interface between vacuum and WSM**

It is possible to determine the free parameter \( \alpha \) if we consider a WSM at \( z \leq 0 \) and also the insulating phase at \( z > 0 \). This can be achieved by modifying the Hamiltonian from Eq. (15) with \( u = u_z \) and \( \chi = 1 \) by replacing \( k_y \) with

\[
\tilde{k}_y(z) = \begin{cases} 
\frac{+k^2 - k_y^2}{2\Delta}, & z \leq 0 \\
\frac{\Delta^2 - k_y^2}{2\Delta}, & z > 0,
\end{cases}
\]

(23)

where \( 2k_0 \) is the distance between the Weyl nodes and \( \Delta > 0 \) the gap of the insulator. On both sides the wave function has to decay exponentially, i.e. we have to fulfill the conditions (I) \( \text{Re}(\lambda) > 0 \) for the WSM and (II) \( \text{Re}(\lambda) < 0 \) on the gapped side for all \( k_\| \). From Eqs. (17) and (21) we find

\[
\text{Re}(\lambda) \propto \sin(\alpha)k_x + \cos(\alpha)\tilde{k}_y(z). 
\]

(24)

Thus, condition (II) is only satisfied for all \( k_\| \) if \( \sin(\alpha) = 0 \) and \( \cos(\alpha) > 0 \), i.e. \( \alpha = 0 \). Condition (I) then requires the surface state to be located at \( |k_y| < k_0 \) and the Fermi arc becomes a straight line between the Weyl nodes. This also holds for the perfect vacuum \( \Delta \to \infty \).

**C Wave function for finite system**

For the finite system we take the same Hamiltonian and ansatz as in the semi-infinite case (Eqs. (15) and (18)), restrict them to \(-L/2 \leq z \leq L/2\), and solve Schrödinger’s equation for \( \lambda \) first. This results in

\[
\begin{align*}
\lambda &= \frac{s\sqrt{k_\|^2 - \epsilon^2 - iu_z\epsilon}}{\sqrt{1 - u_z^2}} \\
\psi &= \frac{1}{\sqrt{2}} \left( \frac{e^{-i\theta}\sqrt{k_\|^2 - \epsilon^2}}{k_\| + ik_y} \sqrt{1 - \chi u_z} \right),
\end{align*}
\]

(25)

(26)

with \( \epsilon(k_\|) \) defined via the energy \( E(k_\|) \) of the surface state as \( \chi \sqrt{1 - u_z^2} \epsilon(k_\|) = E(k_\|) - k_\| \cdot u \) and \( s = \pm 1 \).

Note that this is consistent with the results of the semi-infinite system. The full wave function is a superposition of both solutions of \( \lambda \), i.e.

\[
\Psi(k_\|, z) = \frac{e^{i\theta}r_\|}{\sqrt{2}} \sum_{s=\pm 1} s c_s e^{-\alpha s z} \psi_s
\]

(27)

The condition for hermiticity now is

\[
\psi_1^\dagger(\chi z + u_z) \psi_2 |z = -L/2 = \psi_1^\dagger(\chi z + u_z) \psi_2 |z = +L/2.
\]

(28)

Since our wave function will in general have different weights \( |\Psi(z = +L/2)|^2 \not= |\Psi(z = -L/2)|^2 \) on both surfaces, Eq. (28) can only be satisfied if both sides of the equation are equal to zero. This leads to the same pseudo-spin polarization and wave function at the surface as Eqs. (17) and (22), but the free parameter \( \alpha_t/b \) can be different on top and bottom surface. By using these boundary conditions we find an equation for energy \( \epsilon(k_\|) \):

\[
\tanh \left( L \sqrt{\frac{k_\|^2 - \epsilon^2}{1 - u_z^2}} \right) = \frac{\sqrt{k_\|^2 - \epsilon^2 \cos(\gamma)}}{k_y \cos(\theta) - k_x \sin(\theta) - \epsilon \sin(\gamma)}
\]

(29)

where \( \alpha_t = \theta + \gamma \) and \( \alpha_b = \pi - \theta - \gamma \). For \( \theta = 0 \) normalization yields

\[
\begin{align*}
\epsilon_s^2 &= c_0 \left( (k_x + ik_y \sin(\gamma) - i\epsilon - \sqrt{k_\|^2 - \epsilon^2}) - k_x(k_x + ik_y) \right) \\
\frac{L \epsilon_c^2}{c_0} &= \sqrt{1 - u_z^2} \cos(\gamma) \left( k_y \epsilon - k_\|^2 \sin(\gamma) \right),
\end{align*}
\]

(30)

(31)

\[
\epsilon_0^2 = (\epsilon - k_y \sin(\gamma))^2 - (k_x \cos(\gamma))^2.
\]

(31)

Fig. (3) shows the resulting Fermi arc and hotline in dependence of system size \( L \). To compute the the BC, we
obtained the wave function by numerically solving Eq. \[29\] and taking a finite symmetric difference quotient for the derivatives.

## D Berry curvature dipole for TaAs and TaP

In order to access the parameters for TaAs and TaP, we performed a density-functional (DFT) calculation for these materials using a generalized gradient approximation [25] as implemented in the FPLO code version 48.00-52 [26]. Using 21\(^3\) k-points in a box of length 7\(\times 10^{-3}\) Å\(^{-1}\) around the Weyl point, we fitted the DFT data to the generalized model Hamiltonian

\[ H_G = V k \cdot \sigma + (\mu + u \cdot k) \sigma_0 \]  

where \(\mu\) is the chemical potential and \(V = V^T\) a symmetric velocity matrix with chirality \(\chi = \text{sign(det}(V))\). With an accuracy of 10\(\mu\)eV, this results for TaAs in \(\mu = -8 \mu\)eV and (in units of \(10^5 \frac{m}{s}\))

\[ u = \begin{pmatrix} -0.86 \\ 0.86 \\ 1.44 \end{pmatrix}, \quad V = \begin{pmatrix} 3.38 & 0.84 & 0.88 \\ 0.84 & 2.53 & 0.98 \\ 0.88 & 0.98 & 2.95 \end{pmatrix}, \]  

and the Weyl node is located at

\[ k_W = \begin{pmatrix} 0.039 \\ 0.511 \\ 0.309 \end{pmatrix} \text{ Å}^{-1}. \]  

For TaP we find \(\mu = 6 \mu\)eV and:

\[ k_W = \begin{pmatrix} 0.032 \\ 0.515 \\ 0.314 \end{pmatrix}, \quad u = \begin{pmatrix} -0.86 \\ 0.61 \\ 1.50 \end{pmatrix}, \quad V = \begin{pmatrix} 3.08 & 0.69 & 0.74 \\ 0.69 & 2.29 & 1.11 \\ 0.74 & 1.11 & 2.82 \end{pmatrix}. \]  

The surface state can be solved in the same manner as in the first section. The surface condition changes to \(\mathbf{n} \cdot \nabla \mathbf{s} = -u_z\) and we get

\[ \lambda = k_{||} \cdot \frac{V (\mathbf{s} \times \nabla \mathbf{n}) - i V (\mathbf{n} + u_z \mathbf{s})}{|\nabla \mathbf{n}|^2 - u_z^2}. \]  

A straight-forward calculation yields the BC

\[ \Omega = \frac{\text{Im} (\nabla \lambda) \times \text{Re} (\nabla \lambda)}{2 \text{Re}^2 (\lambda)} \]  

\[ \lambda = \left( \left| \frac{V (\nabla \mathbf{n})^2 - u_z^2}{|\nabla \mathbf{n}|^2 - u_z^2} \right| (V^{-1} \mathbf{s} \cdot \mathbf{n}) \right) \frac{2 \text{det}(V)}{(k_{||} \cdot (V^{-1} \mathbf{s} \times \mathbf{n}))^2} \mathbf{n} \]  

and finally the BCD

\[ D = \frac{|V \mathbf{n}|^2 - u_z^2}{8 \pi^2 \text{det}(V) k_c |V^{-1} \mathbf{s} \times \mathbf{n}|} \cdot \frac{V \mathbf{s} + u \mathbf{n}}{1 + V^{-1} \mathbf{s} \cdot u}. \]  

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