

Step-Edge Anomaly in Topological Metals

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Bulk–boundary correspondence guarantees the presence of robust, anomalous states on the boundary of topological matter. The edges of a two-dimensional Chern insulator harbor one-dimensional chiral states, which have a conductance $n e^2/h$, where n is an integer that is solely determined by the bulk. In this Letter we show that step edges on the surface of three-dimensional topological metals have a robust conductance $K e^2/h$, where K is also fixed by the bulk and assumes noninteger values. We explain this prediction on the basis of the topology of gapless systems, exemplify it on a lattice model, and connect to recent experimental observations of enhanced density of states at step edges in topological metals.

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Introduction—Bulk–boundary correspondence is a unique manifestation of the topology of a bulk material in form of anomalous states on its surface, where the attribute *anomalous* expresses that the surface states cannot exist independently from the higher-dimensional topological bulk [1–4], which, in turn, guarantees the presence and robustness of anomalous surface states given a topological bulk system. This link underpins robust transport properties of the surface, forming the foundation for applications such as in low-dissipation information processing [5,6], and enables the identification of bulk topology from surface phenomena [7,8]. States bound to defects [9–13] can also play this role if the bulk topology is of the “weak” type, but without weak topology, defect-bound states are often only suggestive, rather than implicative, of a topological bulk.

The discovery of novel, unambiguous manifestations of topology on the material surfaces is of great interest as it can substantially expand the application landscape of topological materials as well as tools for identification. Here we predict such an anomalous manifestation at step edges on otherwise featureless surfaces of three-dimensional topological metals, motivated by experimental observations of enhanced and continuous density of states there [14–16]. In topological metals [4,17,18], the bulk is characterized by topologically protected band touching points that resemble the dispersion of Weyl fermions and its various generalizations and come in pairs of

opposite chirality. The corresponding boundary states are open sheets of surface states connecting the projections of opposite-chirality Weyl cones onto the surface Brillouin zone (BZ). The open equienergy contours at the Fermi energy are called Fermi arcs. On surfaces for which the projections of opposite-chirality Weyl nodes overlap, Fermi arcs are absent.

A surface with a Fermi arc has an anomaly that can be quantified in terms of a conductivity. Let the pair of Weyl nodes be separated by $2\pi\mathbf{K}$. The Fermi-arc surface band are chiral surface modes moving in the direction $\mathbf{K} \times \mathbf{e}_s$, where $\mathbf{e}_s$ is the surface normal, for each surface momentum component along $(\mathbf{K} \times \mathbf{e}_s) \times \mathbf{e}_s$ between the projected nodes. Application of a uniform scalar potential $e dV$ at the surface induces the charge-current density $d\mathbf{j} = (e^2/h)\mathbf{K} \times \mathbf{e}_s dV$, where e^2/h is the unit of conductance. The resulting conductivity quantifying the surface anomaly,

$$\sigma_s = \frac{e^2}{h} |\mathbf{K} \times \mathbf{e}_s|, \quad (1)$$

depends only on the separation of the Weyl nodes in the bulk band structure and the surface orientation and is independent of the detailed surface termination. It manifests experimentally as an anomalous Hall conductivity [19,20] in time-reversal broken systems, such as the considered minimal model of two Weyl nodes. In time-reversal-preserved topological metals, Fermi arcs come in countermoving pairs, in which case the longitudinal conductivity contribution of Fermi arcs manifests as inverse resistance scaling [21–27].

In this Letter, we extend this bulk-surface correspondence to a bulk-step-edge correspondence for a step edge in which the surface is shifted by an integer number of unit cells [28]. In particular, we show that a pair of Weyl nodes

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with separation $2\pi K$ gives rise to an anomalous step-edge conductance

$$G_{\text{se}} = \frac{e^2}{h} \nu |\mathbf{K} \times \mathbf{e}_{\text{se}}|, \quad (2)$$

where $\mathbf{e}_{\text{se}}$ is the unit vector normal to the mini surface of the step edge and ν is its height; see Fig. 1(a). The conductance G_{se} can assume a noninteger multiple ($\nu |\mathbf{K} \times \mathbf{e}_{\text{se}}|$) of the unit of conductance. This is different from the anomalous conductance associated with discrete chiral modes, such as in a Chern insulator or a finite Weyl-semimetal surface [19] (see below), which is quantized in integer units of e^2/h . Here we instead show that the fractional response of Eq. (2) is a combination of the quantized response of modes localized at the step edge and a nonquantized local response carried by bulk modes. The number of localized modes at the step edge (if any) depends on local details at the step edge. However, the value of the conductance does not. Note that Eq. (2) is nothing but the application of Eq. (1) to the mini surface of the step edge. However, the total conductance associated with the surface anomaly of Eq. (1) is subject to finite-size corrections, which, e.g., force the net conductance at a finite surface to be quantized [19]. If applied to a surface with a width of a few unit cells, finite-size corrections would be of the same order as the conductance itself. Our prediction is that such corrections are *absent* for the mini surface of a step edge.

Before we detail the mechanism behind the noninteger step-edge conductance, we first use a simple *Gedanken-experiment* [16] to explain its origin in the bulk band structure of the topological semimetal. We consider a model system of Fig. 1(a), but first with a flat upper surface without a step edge. Consider that this upper surface is in the plane that is slightly tilted by an angle θ around the y axis from the constant- z plane. The Weyl node projections onto the new surface BZ will be separated by $K \sin(\theta)$ and the resulting small Fermi arc carries chiral current density $dj_t = dV(e^2/h)K \sin(\theta)$. Since this current only depends on the bulk and the global surface orientation, it is invariant with respect to microscopic modifications of the surface. The tilted surface may thus consist of a periodic sequence of large constant- z plateaus of size L and small steps of height ν with $\nu/L = \tan \theta$. The current per step edge is thus $dI_{\text{se}} = (dj_t) \times L / \cos(\theta) = dV(e^2/h)\nu K$. Since the large constant- z plateau is a surface onto which Weyl nodes project onto one another it does not support a chiral current, so that dI_{se} must be concentrated at the step edge. The step-edge conductance dI_{se}/dV is thus as given in Eq. (2).

While this argument is appealing because of its simplicity, some questions remain: the tilted-surface argument does not resolve contributions of eventual localized modes at the step edge and bulk modes and it does not address the energy window within which the universal step-edge

conductance applies. The size of the energy window matters, because for a tilted surface the Fermi-arc length and, hence, the energy window in which well-defined surface modes exist goes to zero as the tilt angle $\theta \rightarrow 0$. In the calculations below we address these questions by first considering a numerical simulation on a minimal lattice model, followed by an analytical calculation.

Lattice simulation—As a simple model realization of a system exhibiting the step-edge conductance (2), we consider a tight-binding model whose low-energy physics is governed by two Weyl cones of opposite chirality described by the two-band Hamiltonian

$$H = [2 - \cos(k_y) - \cos(k_x) + \cos(\pi K) - \cos(k_z)]\sigma_z + \sin(k_x)\sigma_x + \sin(k_y)\sigma_y, \quad (3)$$

where $\{k_i\}$ are momenta, $\{\sigma_i\}$ denote Pauli matrices, and lattice constants, hopping amplitudes, and $\hbar$ are set to one. The Weyl nodes are located at $k_z = \pm\pi K$. We consider the model (3) on a slab geometry with surfaces perpendicular to the z axis and thickness L_z . Since the projections of the Weyl points onto the surface Brillouin zone coincide, such a surface has no Fermi arc state.

To identify the current carried at step edges, we consider step edges of unit height, running along the y direction, on the top and bottom surfaces. Since the step edges run in the y direction, our system is manifestly translation invariant along y . To avoid Fermi arc states at open boundaries at $x = 0, L_x$, we extend the system periodically along x . The period is L_x plus a shift by ν unit cells along z ; see Fig. 1(b) for $\nu = 1$. Although L_x and L_z must be finite in our numerical calculations, we take them large enough that our results do not depend on them.

We compute the eigenstates of the lattice model at a fixed energy ε for all k_y using the transfer matrix of a finite sized

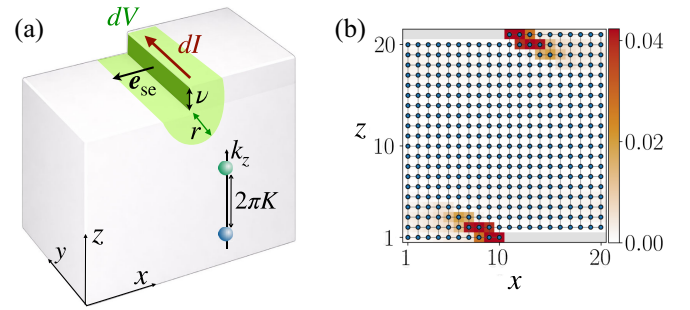


FIG. 1. (a) Weyl semimetal with two Weyl nodes separated by $2\pi K$ in the k_z direction. The upper surface consists of two half planes at constant z , separated by a step edge of height ν . A local potential dV applied at the step edge results in a current response dI in the y direction. (b) Lattice geometry in x and z direction with step edges on top and bottom surfaces for system size $L_x = L_z = 20$ with overlay of local density of states at $\varepsilon = 0.1$ for Weyl node separation of $K = 5/6$. At the top and bottom step edges two states localize.

layer [see Supplemental Material (SM) [29] for more details]. The local density of states shows enhanced weight at both step edges; see Fig. 1(b). We calculate the step-edge conductance $G_{\text{se}} = dI/dV$ by calculating the current dI in the y direction in linear response to a voltage dV applied to a half-cylindrical region within a distance $\leq r$ from the step edge. The current is obtained by summing the y -velocity expectation value $v_{y,n} = \partial E_n / \partial k_y$, where E_n are the energy eigenvalues, over all occupied states, $dI = -e \int dk_y \sum_n v_{y,n} f_n(E_n)$, where $f_n(E_n)$ is the nonequilibrium occupation of the energy eigenvalues. In linear response, the local voltage changes the energy eigenvalues by $\delta E_n = -e dV \int_{x^2+z^2 < r^2} dx dz |\psi_n(x, z)|^2$, where $\psi_n(x, z)$ is the wave function normalized over the (x, z) plane. Hence, the occupation function changes from the Fermi-Dirac equilibrium distribution $n_F(E_n)$ to $f_n(E_n) = n_F(E_n) + n'_F(E_n) \delta E_n$. We set the temperature to zero, in which case the conductance simplifies to

$$G_{\text{se}} = \frac{e^2}{h} \sum_{k_y} \text{sign}(v_{y,n(k_y)}) \int_{x^2+z^2 < r^2} dx dz |\psi_{n(k_y)}(x, z)|^2, \quad (4)$$

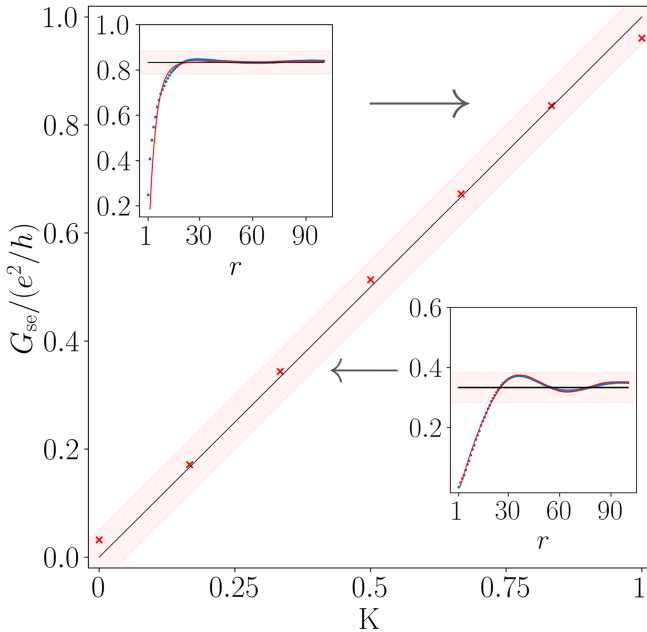


FIG. 2. Step edge conductance (red crosses) as defined in (4) at different values of the Weyl-node separation $2\pi K$ for system size of $L_x = L_z = 400$, step edge of height $\nu = 1$, and energy $\varepsilon = 0.05$. The black line is the universal conductance of Eq. (2). Insets show step edge conductance for $K = 1/3$ and $K = 5/6$ as a function of radius r of the half-cylindrical region in which the potential dV is applied. The red shaded region is a window of width 0.1 to visualize scales between the insets and the main plot. At each K , the numerically calculated response is fitted to a function of the form $f(r) = A(1 - e^{-Br}) + C \sin(D(r - \bar{r}))/((r - \bar{r})^2 + \bar{r}^2)$ to extract the value A of the step edge conductance (for more details, see SM [29]).

where the sum runs over all k_y at which there is a state $n = n(k_y)$ that crosses the (Fermi) energy, $E_{n(k_y)} = \varepsilon$. We find that the conductance does not depend on the energy ε in the energy range of valid Weyl-fermion dispersion (see below); at finite temperature T it will thus saturate to G_{se} of Eq. (4) for $k_B T$ lower than that energy range (k_B being the Boltzmann constant). Figure 2 shows the step-edge conductance at the upper step edge of size $\nu = 1$ as a function of K . We find that, independent of energy and system size, the conductance quickly reaches the predicted value (2), followed by an oscillating tail with a decreasing amplitude $\sim 1/r$. Similar plots are obtained for larger step sizes ($\nu > 1$), different energies, and with surface potential (see below and SM [29] for more data). The values of r at which the conductance is converged does not scale with the system size. Sources of small deviations of the asymptotic values from the expected values are finite-size effects and nonlinear corrections to the Weyl-fermion dispersion. The latter can be expected to be more pronounced at $K = 0$ and $K = 1$ where the two Weyl nodes merge, explaining the larger deviations there. This upper bound does not scale with system size, addressing one of the open questions posed by the tilted-surface argument. At very low energies we find deviations due to finite size effects, which vanish with an increasing system size.

The numerical results confirm that the conductance assumes the expected value $G_{\text{se}} = (e^2/h)\nu K$. It only depends on the bulk property, namely, the separation of the Weyl nodes K . It is instructive to see how the non-quantized current is carried by individual states located near the step edge. Instead of fully localized chiral modes, several bulk states have a strongly enhanced weight near the step edge. This can be seen in the k_y dispersion plotted in the middle panel of Fig. 3, where the spatial inhomogeneity of the states is quantified by the probability-density difference between the upper and lower halves of the lattice. We observe linearly dispersing chiral states confined predominantly to one half of the system, but also additional states at slightly higher energies that are spatially inhomogeneous. Even further inside the cones (both located at $k_y = 0$) the states are homogeneous as expected for bulk states. Note also that the nonquantized value can be attained only if the system is large enough that there are sufficient modes that can carry the nonquantized current. Close to the nodal points this is not the case, which is the finite-size effect at low energies mentioned above.

Effect of a step-edge potential—While the step edge conductance only depends on the bulk parameter K , the distribution of the current among different states and the resulting density of states at the step edge is allowed to depend on surface properties. Indeed, characteristic changes arise if we add a scalar on-site potential on the step-edge sites, the sites on the uppermost and lowermost z layers, next to the step edge. The resulting dispersion is shown in the right panel of Fig. 3. A positive (neg.) scalar

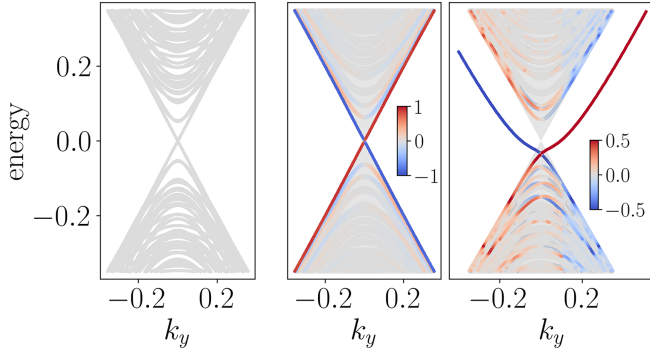


FIG. 3. Dispersion for lattice model for $K = 2/3$ and system size of $L_x = L_z = 50$ with (left) no step edge, (middle) one pair of step edges without, and (right) with an on-site potential $V = -0.6$ at the step edges. The coloring shows the difference in density of states, with positive (red) and negative (blue) corresponding to larger d.o.s. in the top and bottom halves of the system, respectively. The potential splits off one chiral mode at each step and pushes it into the bulk gap, while bulk modes of opposite velocity localize at the step. In gray we color the bulk cone of an infinite system without step edge.

on-site potential next to the step edge pushes states localized at the step edge to higher (lower) energies while bulk states remain unaffected. As a result, the localized parts of the states on the lower (upper) dispersion branch split off and form fully localized states within the k_y -dependent energy gap. This fully localized in-gap state contributes (e^2/h) to the conductance, independent of K . This alone would violate the predicted step-edge conductance of $(e^2/h)K$. However, at the same energies, bulk states of *opposite velocity* partially localize at the step edge, as can be seen in the plot, so that the total conductance is kept at the universal value of Eq. (2), independent of the potential. A qualitatively similar effect occurs if the potential is added to the whole surface (not shown). The potential leads to a strongly enhanced local density of states at energies to one side of the Weyl nodes (see SM [29] for a quantitative plot). Such a characteristic asymmetric density at step edges around the Weyl nodes agrees with the experimental observation in Ref. [16].

Analytical calculation of the step-edge conductance—As an alternative analytic derivation of the step-edge conductance, we consider a WSM with N unit cells in the z direction and let the Weyl nodes projected onto the constant- x surface be at $k_z = \pm\pi K$. The eigenstates are standing waves with quantized momenta $k_{z,l} = l\pi/(N+1)$, $l = 1, \dots, N$. A termination in x direction generates exponentially localized Fermi arc states at $k_{z,l} < \pi K$. The x -dependent part of the Fermi-arc wave function close to a node, where the Hamiltonian can be expanded to linear order in the x momentum, is of the form

$$\psi_{k_{z,l}}(x) = \sqrt{2\Delta(k_{z,l})} e^{-\Delta(k_{z,l})x}, \quad (5)$$

where $\Delta(k_{z,l})$ denotes the inverse localization length, which is proportional to the bulk gap, and the prefactor ensures normalization. We assume a well-defined Weyl semimetal with a bulk gap between the nodes ($k_{z,l} \sim 0$) on the order of $1/K$ and smoothly approaching zero at $k_{z,l} = \pi K$. The current dI induced in response to a surface potential $-e dV$ applied in a region of length r from the surface is obtained by summing over all Fermi arc states the probability density integrated in x over the interval $[0, r]$. For $r \gg 1/K$, almost all Fermi arc states, except those close to the Weyl nodes, are fully localized within the region, so that the integral is unity for those states, which justifies consideration of wave functions close to the nodes, only. The induced current thus reads

$$dI_N = dV \frac{e^2}{h} \sum_{l=1}^{l_{\max}} (1 - e^{-2\Delta(k_{z,l})r}), \quad (6)$$

$k_{z,l_{\max}}$ being the largest momentum satisfying $k_{z,l} < \pi K$. We now consider two copies of this finite slab with $N+1$ and N layers along z , respectively, placed next to each other such that one of the slabs has one more layer on the top, as shown in Fig. 4. When uncoupled, the two slabs give rise to the chiral surface currents dI_{N+1} and $-dI_N$ at the interface. A straightforward calculation of the total interface current $dI \equiv dI_{N+1} - dI_N$ under the assumption $r \ll N$ leads to

$$dI = dV(e^2/h)K \quad (7)$$

(see SM [29] for a detailed calculation). To connect this result with the current carried by a step edge, we consider what happens upon introducing a local hopping at the interface between the two slabs, which would merge the two slabs into a single slab with a step edge on the top surface as displayed in Fig. 4. While the two interface surfaces are modified by the introduced hopping, the total current response dI is unchanged. This can be seen by considering that application of dV on the outer opposite surfaces of the two slabs would compensate the interface-induced current dI . If the local hopping at the interface would modify dI it would modify the response at the outer surfaces as well, which contradicts the locality of the hopping-amplitude change. The interface hopping can thus be chosen such that the interface disappears and the upper and lower surfaces become featureless, except for the step edge on the upper surface. Since the featureless surfaces do not support a current response in the y direction, the current response dI must be uniquely associated with the step edge.

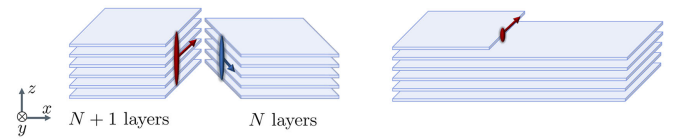


FIG. 4. (Left) Two slabs with $N+1$ and N layers in z direction. (Right) The two slabs coupled into a single slab with a step edge on the top surface.

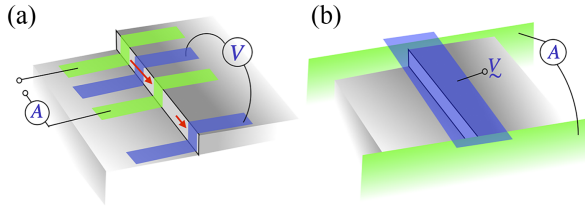


FIG. 5. Schematics of possible experimental setups to detect chiral step-edge conductance. (a) Four-terminal setup. (b) Three-terminal setup with ac voltage bias.

Note that this analytic calculation of the step-edge conductance is valid also at energy $\varepsilon = 0$, which was inaccessible numerically due to the finite size.

Discussion—The noninteger step-edge conductance $G_{\text{se}} = (e^2/h)(\nu|\mathbf{K} \times \mathbf{e}_{\text{se}}|)$ is universally determined by the separation of a pair of Weyl nodes in the bulk and the step-edge orientation. In case of multiple Weyl-node pairs and additional nontrivial bulk topology, all contributions add up independently, whereby the noninteger part of G_{se} related to the positions of the Weyl node pairs, derived here, can be supplemented with an integer part, associated with the topology characteristic of a three-dimensional (stacked) Chern insulator.

Although the experimental verification of the step-edge conductance requires transport measurements, some qualitative properties of the local density of states detected in [16] are consistent with our theory: the density of states is observed to have an asymmetric energy dependence around the Weyl nodes, which we identified as a hallmark of a chiral state separated from the bulk continuum by a generic local potential at the step edge. Furthermore, the density of states along the step edge observed in [16] remains remarkably smooth despite evident surface disorder, which one can understand as prohibited standing-wave formation when the weights of forward- and backward-moving wave functions are different. In the presence of disorder, we expect that the chiral step-edge currents enjoy the same robustness as the currents carried by Fermi arcs on extended disordered surfaces of topological metals [31]. When interactions become strong enough to overcome topological protection of Fermi arc states, we expect the step-edge conductance to lose its robustness as well [32–34].

Interesting for future experiments is a direct detection of the step-edge anomaly. This can be achieved in magnetic topological metals in a four-terminal setup, measuring a voltage difference between two parts of the step edge, one of which conducts a current, illustrated in Fig. 5(a). A quantitative measurement of the noninteger step-edge conductance can be achieved by applying a local ac voltage bias along the step and collecting the resulting current flow by leads, as illustrated in Fig. 5(b). Such experimental probes of Weyl topology are especially valuable in systems where opposite-chirality Weyl nodes project onto one another on the natural surfaces, such as $(\text{Cr}, \text{Bi})_2\text{Te}_3$

[35], EuCd_2As_2 [36,38], and MnBi_2Te_4 [39]. In these materials, the overlapping surface projections preclude the conventional surface signatures of Weyl topology, making the step-edge signature proposed here a unique manifestation of the underlying topological phase.

In closing, it is interesting to point out that the robust step-edge conductance could play an important role in the mechanism of record-low resistivity measured in topological-metal nano-structures [21,27]. Their boundaries naturally feature step edges that, depending on the sample geometry and the density of step edges, could dominate the transport. Generally, in combination with emerging microstructuring capabilities [40], our discovery of one-dimensional chiral transport channels on surfaces of stable three-dimensional matter opens a new route for harnessing robust transport in quantum electronics.

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Data availability—All the code and data used to produce the reported results is available in Ref. [41].

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