

1 Classification of Weyl points

Type II Weyl points occur when type I Weyl nodes are tilted enough – along some specific direction – that a Lifschitz transition occurs and the system acquires finite density of states at the Weyl node. Although several possibilities of small tilting of the Weyl cone were discussed in some works [1, 2, 3, 4, 5], none of these works pointed out the Lifschitz transition that gives rise to a fundamentally new type of Weyl fermion, with new thermodynamic properties. Given the existence of at least two types of Weyl fermions, we can ask if any other types of Weyl points can exist. In the present section we show that a mathematical theorem states that only two types of Weyl points are possible, and hence our classification is complete.

The most general linear in $\mathbf{k}$ Hamiltonian of a Weyl point is

$$H(\mathbf{k}) = \mathbf{v} \cdot \mathbf{k} + \sum_{i,j=1}^3 k_i A_{ij} \sigma_j \quad (1)$$

where A is a 3×3 matrix and σ 's are the Pauli matrices. The Fermi surface for the chemical potential μ can be obtained by solving the equations $\epsilon_{\pm}(\mathbf{k}) = \mu$, where

$$\epsilon_{\pm}(\mathbf{k}) = \mathbf{v} \cdot \mathbf{k} \pm \sqrt{\sum_{i,j} k_i [AA^T]_{ij} k_j} \quad (2)$$

are the two eigenvalues of the Hamiltonian. By squaring the Eq. 2 the Fermi surface can be shown to be satisfied on the quadric surface described by the following equation

$$\sum_{i,j} k_i ([AA^T]_{ij} - v_i v_j) k_j + 2\mu \mathbf{v} \cdot \mathbf{k} - \mu^2 = 0 \quad (3)$$

Classification of all possible quadric surfaces is known [6]. Applying this classification to the equation above one can show that there only two possible types of Weyl points: type-I with a closed point-like Fermi surface, and type-II with an open Fermi surface, as described in this paper. The classification [6] also gives rise to different kinds of nodal lines and surfaces, which will be the subject of further study [7].

2 Transport signatures of type-II Weyl semimetals

Here we show that the transport properties of the two different types of Weyl points are very distinct. In particular, the type-II Weyl points give rise to a new kind of chiral anomaly. Here we report the main conclusions, and a more detailed explanation will be presented elsewhere [8]. We also discuss another difference between the two types of Weyl points, which appears in the density of states, leading to very different thermodynamic properties.

2.1 Novel chiral anomaly in type-II Weyl semimetals

Let us consider the Hamiltonian

$$H(\mathbf{k}) = Ck_z + \mathbf{k} \cdot \boldsymbol{\sigma} \quad (4)$$

which realizes a Weyl point with a +1 Chern number. The type of this Weyl point depends on the value of the parameter C , being of type-II for $|C| > 1$ and of type-I otherwise. This Hamiltonian is a much simplified version for that of a type-II Weyl, but has the advantage of being analytically tractable in some limits and will be used for qualitative purposes.

If a magnetic field of magnitude B is applied along the $\hat{z}$ -direction the spectrum of the Landau levels is given by

$$E_n^\pm = Ck_z \pm \sqrt{k_z^2 + \frac{2n}{\ell^2}} \quad (5)$$

where $\ell = (eB/c)^{-\frac{1}{2}}$ is the magnetic lengthscale, e is the charge of electron, c is the speed of light, and $n > 0$. The 0-th Landau level has the energy

$$E_0 = (C + 1)k_z \quad (6)$$

and is unpaired (chiral). The sign of the electron velocity associated with the 0-th Landau level is given by the sign of $(C + 1)$, as explained below.

If the electric field is applied in the same direction as the magnetic field, chiral electrons start flowing in the $\hat{z}$ -direction. Since Weyl points come in pairs of opposite Chern numbers, the low-energy spectrum of a Weyl semimetal will also host an antichiral 0-th Landau level at the position of the opposite Chern number Weyl point. The current then appears flowing from one Weyl point to another [9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19]. This is a realization of the Adler-Bell-Jackiw chiral anomaly [20, 21] of the quantum field theory in the lattice system [22]. Observation of this effect was reported recently in Dirac semimetals and in the TaAs type-I Weyl semimetal family [23, 24, 25]. For the type-II Weyl semimetal similar behavior is expected for the field applied in the direction of dominating kinetic term, when the spurious large trivial almost compensated Fermi surfaces that exist in the material are discounted and the Weyl contribution is singled out.

A drastic difference between the two types of Weyl points described by Eq. 4 arises when the magnetic field is applied along the $\hat{x}$ -direction, that is in the direction, in which the kinetic term *does not* dominate in the case of $|C| > 1$. For the type-I the above discussed chiral anomaly still appears. For the type-II case of $|C| > 1$, however, the Landau level spectrum becomes gapped and no chiral anomaly can be observed, as illustrated in Figs. 1-2 ($\frac{\sqrt{2}}{\ell} = 0.1$ in all the illustrations).

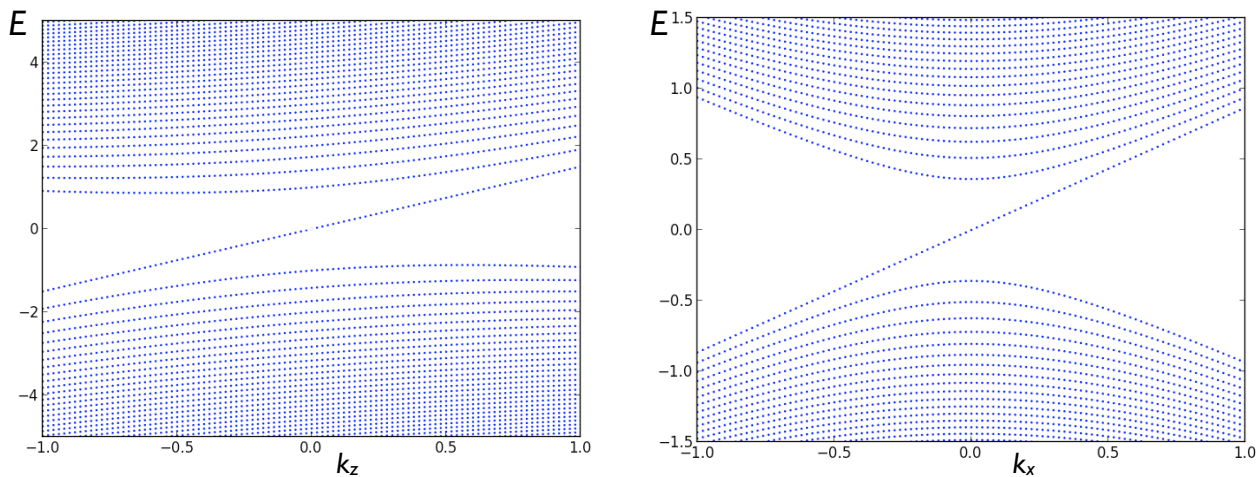


Figure 1: Landau level spectrum for the type-I Weyl point of Eq. 4 with $C = 0.5$. Left panel: the magnetic field is applied along the $\hat{z}$ -direction. Right panel: the magnetic field is applied in the $-\hat{x}$ direction. The chiral 0-th Landau level is present in both cases.

This is easily understood in the limit $C \rightarrow \infty$ by solving the $H = Ck_z$ hamiltonian in a $B||\hat{x}$ field. In a more general case, a long analytic calculation [8] proves the absence of a chiral mode for $B||\hat{x}$ and $C > 1$. In fact, when the field direction is rotated from $\hat{z}$ to $\hat{x}$ the chiral Landau level persists until the angle θ between the field the $\hat{z}$ -axis, becomes such that $\cos^2 \theta = 1/C^2$. For the directions, where $\cos^2 \theta < 1/C^2$ the chiral Landau level disappears.

This situation is generic in type-II Weyl points. The chiral Landau level appears only when the magnetic field is applied in the direction, along which the kinetic term is dominant. If the field is applied in the other direction – no chiral Landau level appears. This dependence of the presence or absence of the chiral anomaly on the direction of the applied magnetic field is the main difference between the two types of Weyl semimetals, with immediate consequences for the transport properties.

There is one more important feature of the type-II Weyl points that does not appear in the type-I case. This is the possibility for the velocity of the chiral Landau level to be *locally* in k -space different from the chirality dictated by the Chern number of the Weyl node. As an example, consider the Weyl point of the Hamiltonian 4. The Chern number of this point is positive, however, for $C < -1$ the velocity of the chiral Landau level appearing in the $\hat{z}$ -field becomes negative as illustrated in the left panel of Fig. 3.

However, this anti-chiral effect is a feature of the linearized Hamiltonian. In a real semimetal higher order terms must exist, responsible for closing the Fermi surface of the type-II Weyl point. These terms will correct the chirality of the Landau level far from the Weyl point as illustrated in the schematic plot in the right panel of Fig. 3.

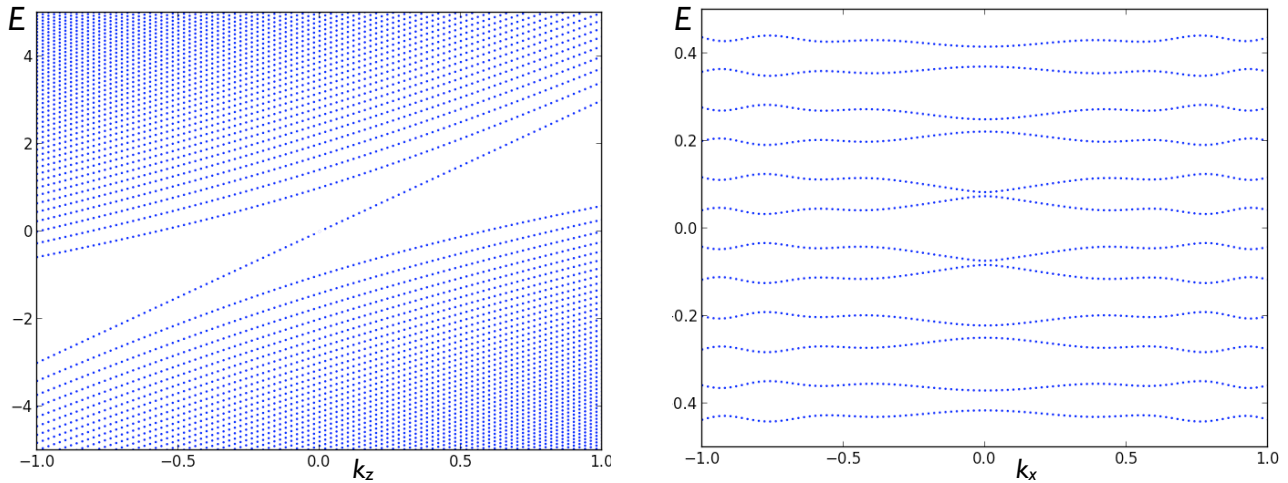


Figure 2: Landau level spectrum for the type-II Weyl point of Eq. 4 with $C = 2$. Left panel: the magnetic field is applied along the $\hat{z}$ -direction. The chiral 0-th Landau level is present. Right panel: the magnetic field is applied in the $-\hat{x}$ direction. No chiral Landau levels exist.

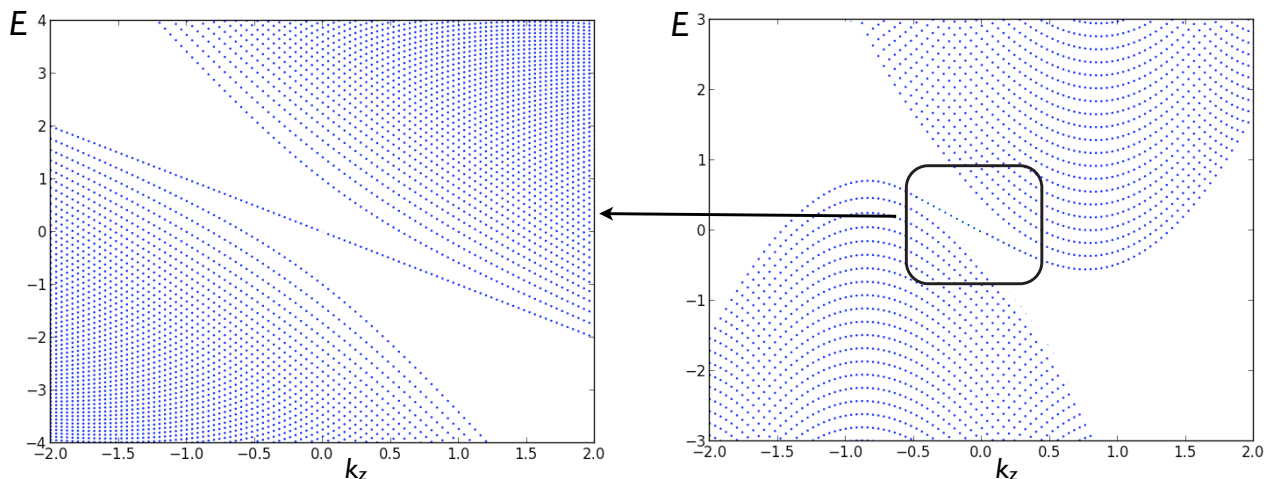


Figure 3: Chirality change at small k_z . Left panel: Landau level spectrum for the type-II Weyl point of Eq. 4 with $C = -2$. The 0th Landau level appears to be a left mover for a Weyl point with Chern number +1. Right panel: Schematic plot based on on a possible realization of the closure of the Fermi surface. The paradox is resolved, when higher-order in k terms are added to the Hamiltonian to close the Fermi surface. These higher order terms render the chirality of the full region to +1. The chiral band is a right-mover with the velocity changing twice at small values of k_z . The framed region is that, where chirality is changing around small k_z .

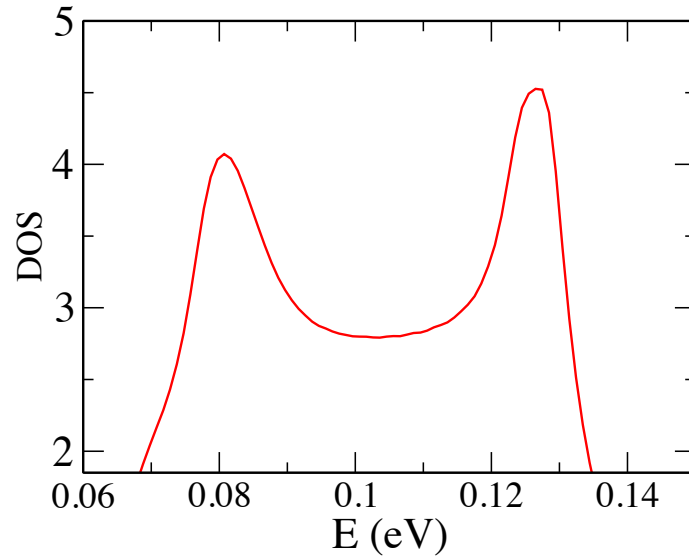


Figure 4: The density of states of the pair of Weyl points in WTe₂. The contribution of the rest of the Fermi surface is not included.

2.2 Thermodynamics of type-II Weyl points

Another significant distinction of the two types of Weyl semimetals appears in the thermodynamic properties. For the type-I Weyl point, described by the Hamiltonian of Eq. 4 the density of states $g(E)$ behaves like

$$g(E) \propto \frac{E^2}{(1 - C^2)^2} \quad (7)$$

For the type-II this behavior changes and the corresponding density of states becomes

$$g(E) \propto \frac{1}{|C|} \left(p_0^2 - \frac{E^2(C^2 + 1)}{(1 - C^2)^2} \right) \quad (8)$$

The constant term p_0 arises due to the presence of unbounded (in the linearized model) electron-hole pockets, and it depends on the cutoff. Due to this term the density of states always remains positive. These formulas were verified versus numerical simulation of the Hamiltonian 4.

To illustrate this claim further we plot the density of states that arises due to the pair of Weyl points in WTe₂ in Fig. 4. The contribution of the rest of the Fermi surface to the density of states is not included. The two clearly visible parabolic peaks in the density of states are due to the two type-II Weyl points. The difference in the energy position of the peaks and the energy of Weyl points reported in the main text is due to the difference between the tight-binding model used here with the actual first-principles calculation. The peaks correspond to the energies of Weyl points in the tight-binding model used to generate Fig. 4.

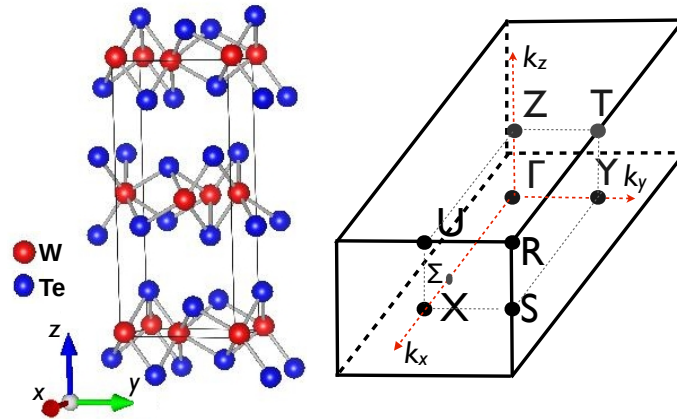


Figure 5: Left panel: crystal structure of WTe_2 . Right panel: Brillouin zone of the rhombohedral unit cell.

3 Crystal structure and computation details

The crystal structure of WTe_2 and its Brillouin zone are illustrated in Fig. 5. Several crystal structures are reported in the databases [26, 27]. We use the latest one from the work of Ref. [27] that was obtained at the lowest temperature. That work explicitly explains minor differences with the earlier works [26] by the higher temperatures in those measurements.

For completeness, we list the experimental structural parameters taken from Ref. [27] that were used in this work. The lattice constants are $a = 3.477$, $b = 6.249$ and $c = 14.018$, and both W and Te atoms occupy $2a$ Wyckoff positions corresponding to $(0, y, z)$ and $(1/2, -y, z + 1/2)$. Values of x and y for this structure are listed in Table 1.

	W(1)	W(2)	Te(1)	Te(2)	Te(3)	Te(4)
y	0.60062	0.03980	0.85761	0.64631	0.29845	0.20722
z	0.5	0.01522	0.65525	0.11112	0.85983	0.40387

Table 1: Positions of atoms in the unit cell of WTe_2 given as coordinates for Wyckoff positions $2a$ of the $Pnm2_1$ space group. Bracketed numbers following the element symbol indicate distinct Wyckoff positions. There are two distinct Wyckoff positions for W and four for Te atoms.

Band structure calculations (both with and without spin-orbit coupling (SOC)) were performed in VASP [28] *ab initio* code using PAW [29, 30] pseudopotentials with $6s^25d^4$ and $5s^25p^4$ valence electron configurations for W and Te correspondingly. The PBE [31] approximation was used. Spin-orbit coupling was implemented in pseudopotentials. The energy cutoff was taken to be 260eV. Gaussian smearing of width 0.05eV and a $12 \times 10 \times 6$ Γ -centered k -point mesh were used to perform Brillouin zone integrations. The conclusions of the paper were also verified using a more elaborate pseudopotential for W with semicore p -states included in the valence, that is with $5p^66s^25d^4$ valence electron configuration.

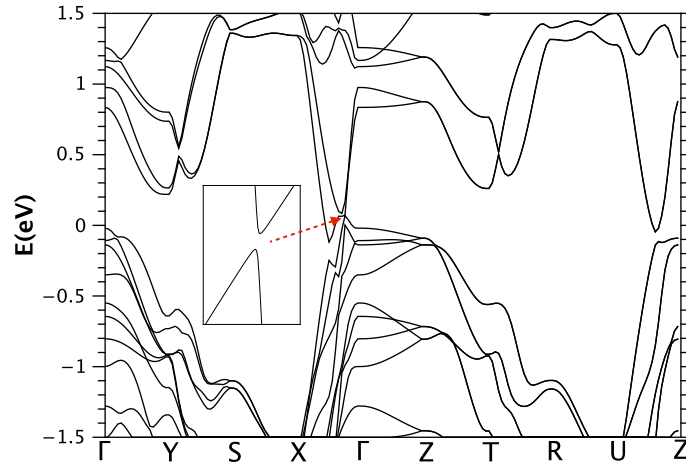


Figure 6: Band structure of WTe₂ without SOC. E_F is set to 0.

4 Electronic structure without spin-orbit coupling

The band structure of WTe₂ in the absence of SOC is shown in Fig. 6. To understand the nature of crossings in this case we carried out an extensive symmetry analysis that will be reported elsewhere [7]. Here we only state the main conclusions. Using a two band model

$$H(k_x, k_y, k_z) = \varepsilon(k_x, k_y, k_z) + \sum_{i=x,y,z} d_i(k_x, k_y, k_z) \sigma_i, \quad (9)$$

where σ_i are the Pauli matrices, one can show that on the $k_z = 0$ plane only two of the three d_i coefficients are linearly independent. The degeneracy occurs if for some (k_x, k_y) both of these coefficients vanish. Thus, there are two independent constraints on two functions of k_x, k_y , the codimension is zero, and the solution is in general possible at isolated points in the $k_z = 0$ plane. In addition, it can be shown that without SOC no band crossings can generally occur along the $\Gamma - X$ axis. Indeed, *ab initio* results show that a small band gap exists in the band structure along $\Gamma - X$, as illustrated in the inset of Fig. 6.

First-principles calculations support our conclusions. Without SOC we find 8 Weyl points (not accounting for spin) in the $k_z = 0$ plane. In addition, we find 8 more spinless Weyls at low symmetry points $k_i \neq 0$ for all i . The coordinates of Weyl points and their Chern numbers are given in Tab. 2.

Now, when spin is taken into consideration but SOC is still neglected, each Weyl point becomes doubled, with doubled chirality due to SU(2) symmetry. When SOC is gradually increased the Weyl points split and start moving in the Brillouin zone. For a material with weak SOC, one can expect this motion to be the only effect of SOC, so that the Weyl points do not vanish in general. In WTe₂, however, SOC is large. To see its effect on the structure of Weyl points in the BZ, we carried out a smooth interpolation between no SOC and full SOC band structures. In the process, other Weyl points appear and disappear (by merging points with opposite chiralities), so that the final arrangement of Weyl points reported in the main text cannot be understood in terms of rearranging the Weyl points that are present in the absence of SOC.

	k_x	k_y	k_z	C
1	0.1054	0.0087	0	+1
2	0.1742	0.1200	0	+1
3	0.14992	0.07845	0.2329936	-1
4	0.14992	0.07845	-0.2329936	-1

Table 2: Coordinates and Chern numbers of 4 out of 16 Weyl points appearing without SOC. The other 12 points are related by the ones listed by reflections being located at $(-k_x, k_y, k_z)$, $(k_x, -k_y, k_z)$ with Chern numbers $-C$ and at $(-k_x, -k_y, k_z)$ with Chern number C . Points at $k_z \neq 0$ are symmetric about the xy -plane due to the compound symmetry formed by time reversal and two-fold rotation.

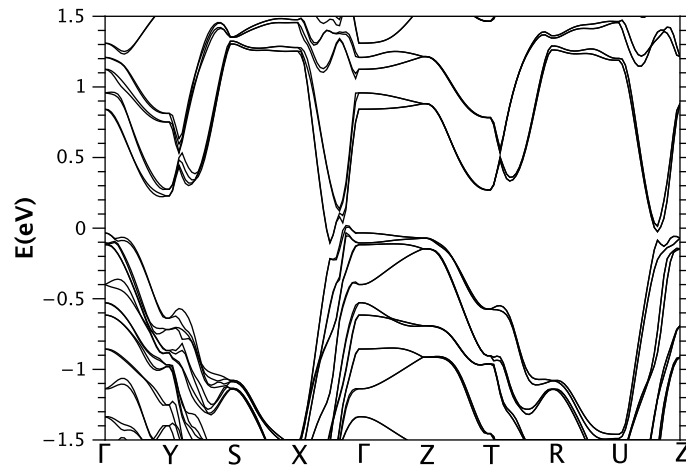


Figure 7: Band structure of WTe₂ with SOC taken into account. E_F is set to 0.

5 Electronic structure with spin-orbit coupling

The fully relativistic band structure is illustrated in Fig. 7. Symmetry considerations indicate the possibility to have locally stable point-like degeneracies in the $k_z = 0$ plane, where a little group formed by a combination of a two-fold rotation and time-reversal exists [7]. As will be explained elsewhere in detail, this suggests that double degeneracies can occur at isolated points in the $k_z = 0$ plane.

In accord with this argument, eight Weyl points (listed in Tab. 3), described in the main text, are indeed located in the $k_z = 0$ plane. A general form of the Hamiltonian around a Weyl point in the $k_z = 0$ plane can be constructed using the following two dimensional representation for the combination of C_2 and time-reversal

$$C_{2T} = -i\sigma_z K \quad (10)$$

where K is complex conjugation. This form of the symmetry can be shown to be consistent with the representations of other symmetries in this non-symmorphic space group.

Keeping only terms linear in k and subjecting the Hamiltonian to this symmetry we find the

	k_x	k_y	k_z	C
1	0.12184	0.03825	0	+1
2	0.12141	0.0454	0	-1

Table 3: Coordinates and Chern numbers of 2 out of 8 Weyl points appearing with SOC. The other 6 points are related by the ones listed by reflections, being located at $(-k_x, k_y, k_z)$, $(k_x, -k_y, k_z)$ with Chern numbers $-C$.

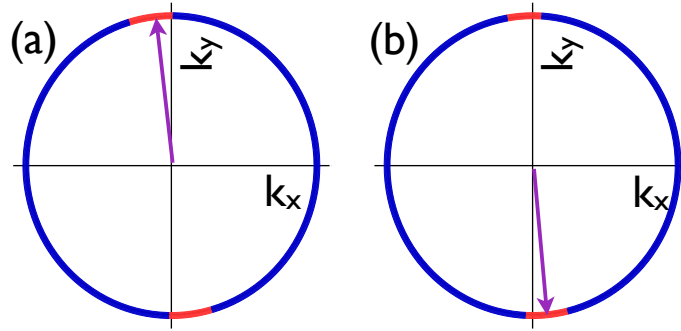


Figure 8: The ratio R of Eq. 13 for the circle of radius 10^{-3} drawn around the two Weyl points. Red color corresponds to $R > 1$, while blue is $R < 1$. The arrows show the direction from one of the two points to the other. Panel (a): Weyl point at $(0.12184, 0.03825, 0)$. Panel (b): Weyl point at $(0.12141, 0.0454, 0)$.

general form of the Hamiltonian around a Weyl point in $k_z = 0$ with SOC

$$H(\mathbf{k}) = \epsilon(\mathbf{k}) + (ak_x + ck_y)\sigma_y + (bk_x + dk_y)\sigma_z + ek_z\sigma_x \quad (11)$$

where

$$\epsilon(\mathbf{k}) = Ak_x + Bk_y \quad (12)$$

For the Weyl point to be of type II, the kinetic part of the energy should dominate over the potential one in at least some direction in k -space. To find such directions for the points in question, we plotted the ratio

$$R = \frac{(Ak_x + Bk_y)^2}{e^2k_z^2 + (ak_x + ck_y)^2 + (bk_x + dk_y)^2} \quad (13)$$

on the circles defined by $k_x^2 + k_y^2 = 10^{-6}$, where k_x and k_y are taken in reduced coordinates, and the constants are explained in the main text. The results are illustrated in Fig. 8. The region, where $R > 1$, meaning that the kinetic energy dominates and the Weyl points are of type II, is shown in red.

Finally, we fitted the Hamiltonian of Eq. 11 to the first-principles band structure around the Weyl points to get the values of its parameters. They are provided in Tab. 4.

point	A	B	a	b	c	d	e
1	-2.739	0.612	0.987	1.107	0.0	0.270	0.184
2	1.204	0.686	-1.159	1.046	0.0	0.055	0.237

Table 4: Parameter values for the Hamiltonian of Eq. 11 around the two Weyl points given in [eVÅ]. Point 1 refers to the Weyl at (0.12184, 0.03825, 0), while point 2 is (0.1241, 0.0454, 0).

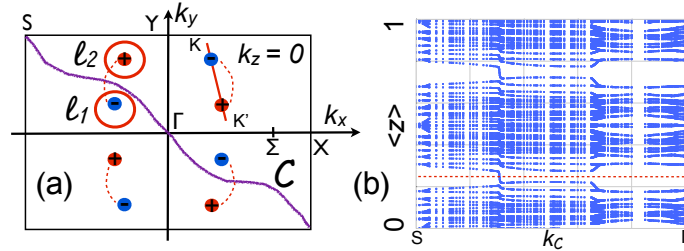


Figure 9: Weyl points of WTe₂. Panel (a): schematic illustration of the BZ cross-section at $k_z = 0$ and Weyl points in it, their chirality marked with red and blue color, corresponding to $C = +1$ and $C = -1$. The red line corresponds to the BZ segment shown in Fig. ??(c). Panel (b): Wannier charge centers (Wilson loop) on the plane, shown schematically as contour C in panel (a). It corresponds to a non-trivial $\mathbb{Z}_2$ invariant.

6 Weyl Nodes and Topological Indices

To rigorously establish the degeneracies of WPs, we examine the structure of the Berry curvature $\mathcal{F}(\mathbf{k})$ of Bloch states around the gapless points. Since a WP represents a monopole in Berry curvature, the flux of $\mathcal{F}$ through a surface enclosing it in k -space is quantized to the total topological charge enclosed, and the FS of WP1, being a closed surface, has non-zero Chern number. In case of WP2, however, the FS is open, and cannot be used to compute its topological charge. Instead, we integrate the Berry curvature of N bands, where N is the number of electrons per unit cell. A surface, on which these N bands have an energy gap to the higher energy bands and which encloses the WP2 can always be found and is used to compute the topological charge of a WP2, as illustrated below.

For WTe₂ these surfaces were taken to be spheres enclosing the Weyl points; see ℓ_1 and ℓ_2 in Fig. 9(a). For the sphere ℓ_1 the Chern number is found to be $C = -1$, proving the existence of a WP of negative chirality inside it. The sphere ℓ_2 , enclosing the second WP, is found to have $C = +1$. This calculation combined with the use of symmetries maps out the structure of the eight WPs in the BZ of WTe₂. They are sketched in Fig. 9(a).

To understand which pairs of Weyl nodes are connected by the Berry flux, thus elucidating the structure of the surface Fermi arcs, several topological invariants are computed from first-principles calculations. TR allows the computation of the $\mathbb{Z}_2$ -invariant [32] on TR-symmetric planes in the BZ, defined by $k_i = 0, \pi$, where $i = x, y, z$. One such plane, the $k_z = 0$ one, hosts WPs, and does not have a well-defined invariant. For the other five planes, where the $N = 72$ bands are gapped from the band $N + 1$, the topological invariant is computed using a hybrid Wannier centers technique [33] and found to be trivial. The corresponding Wilson loops [34] are gapped.

A non-trivial TR $\mathbb{Z}_2$ topological invariant can, however, be defined for WTe₂. It describes the motion of Wannier charge centers on a curved surface that crosses neighboring WPs, as shown by contour $\mathcal{C}$ in Fig. 9(a) where we plot its projection onto the (k_x, k_y) -plane - the surface extends through the BZ in the k_z -direction. If the curve passes through a point (k_x, k_y) then it passes through its TR-image $(-k_x, -k_y)$ as well and the surface satisfies the conditions of the $\mathbb{Z}_2$ -pump [35]. We calculate $\mathbb{Z}_2$ invariant on this surface directly from first-principles calculations using the Z2Pack software [36]. Fig. 9(d) shows that pumping in this plane occurs between two TR invariant momenta: $k_x = k_y = -\pi$ (S) and $k_x = k_y = 0$ (Γ). Thus, the plane $(\mathcal{C}, k_z)$ exhibits a quantum spin Hall effect. If an open surface in the z -direction is introduced, helical surface states appear along the curve $\mathcal{C}$ in the surface BZ, becoming part of the Fermi arcs. As the $k_{x,y} = 0, k_z$ planes have gapped Wilson loops, we conclude that the Berry flux connects pairs of neighboring WPs, as illustrated in Fig. 9(a). This calculation gives another proof that WPs exist in WTe₂, resolving their connectivity and the location of Fermi arcs.

6.1 Computation of chiralities of type-II Weyl points

The Fermi surface of a type-II Weyl point is open, so it cannot be used for integrating the Berry curvature in chirality computation. Instead, the Berry curvature of N bands, where N is the number of electrons per unit cell, should be integrated over a surface, on which these N bands are separated by an energy gap from the higher energy ones. Since the crossing of the N th and $N + 1$ th bands occurs at a point (Weyl point), such a surface enclosing the type-II Weyl point always exists. The calculation becomes equivalent to the usual integration over the occupied bands, if one allows for a k -dependent chemical potential, located in between the N -th and $N + 1$ -th bands at each k -point on the surface.

Following this prescription and using a Wannier function-based tight-binding model [37, 38] described below, Bloch states were calculated on the spheres around the gapless points. The Hamiltonian remained gapped in the above sense ($N = 72$) everywhere on these spheres, schematically illustrated as $\ell_{1,2}$ in Fig. 3(a) of the main text. The corresponding flux of Berry curvature was computed by discretizing a closed sphere, parametrized by angles θ and ϕ , into 1D-loops, as shown in Fig. 10(a). When traversed around a loop, the occupied Bloch states accumulate a Berry phase, the trace of which is computed for each of these loops θ_i using the methods of Refs. [39, 33, 34].

These Berry phases correspond to the average position of charge [40], associated with the bands below the gap, on the loop, $\langle \varphi \rangle(\theta_i)$. Since 1D loops cover a closed surface, the center of charge $\langle \varphi \rangle$ can only shift by an integer multiple of 2π when θ varies from 0 to π . This multiple is equal to the monopole charge enclosed and gives the chirality of the WP enclosed. Similar considerations are used when computing Chern numbers of insulators, with the only difference that the BZ in that case is a torus, rather than a sphere. The result of such a calculation is equivalent to taking the surface integral of the Berry curvature over a closed surface. A more detailed account of this type of calculations, along with the rigorous derivation can be found in Ref. [?]].

The results obtained for WTe₂ is shown in Fig. 10(b) for the sphere ℓ_1 of Fig. 3(a) of the main text. The charge center shifts downwards, corresponding to Chern number $C = -1$, thus proving the existence of a WP of negative chirality inside ℓ_1 . For the sphere ℓ_2 , enclosing the second Weyl point, the Chern number is $C = +1$, and hence the chirality of this point is positive.

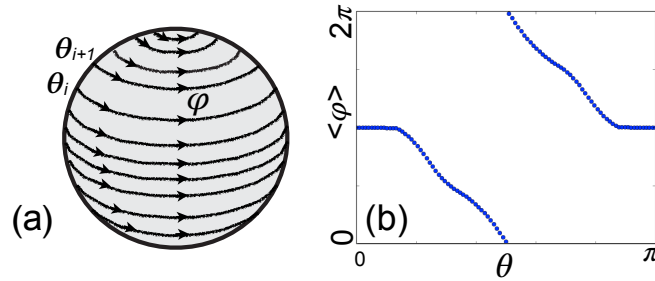


Figure 10: Panel (a): schematic illustration of the integration paths used to calculate topological charges of Weyl points. Panel (b): motion of the center of charge around the sphere is shown schematically for ℓ_1 in panel (a) of Fig. 3 of the main text. The Chern number of the enclosed Weyl point is equal to -1 .

7 Strain effects in WTe_2

As mentioned in the main text, the hydrostatic compressive strain (applied pressure) of 2% increases the separation of the Weyl nodes from 0.7% to 4% of the reciprocal lattice constant separation of the nearest Weyl points. Other strains were also studied. Here we present the summary of the results obtained.

Compressive uniaxial strain along the x -direction also increases the separation between the nearest Weyl points. At 1% strain the separation is 2.2% of $|G_2|$. Further increase of this strain makes one of the two points hit the mirror plane (at $\approx 2\%$ strain), where it is annihilated with its mirror image of opposite chirality, and thus only four Weyl points are left in the $k_z = 0$ plane, all of them being of type-II. This situation, illustrated in Fig. 11, possibly realizes the simplest situation in time-reversal symmetric Weyl semimetals with the minimal number of Weyl points.

The situation changes for the uniaxial compressive strain in the z -direction. While the neighboring Weyls still move further from each other (4.3% of $|G_2|$ for a 2% strain), they both move further away from the mirror plane, so the scenario of only four Weyl points left is not realized in this case. However, we find that this strain drives a phase transition from type-II to type-I Weyl points for four out of eight points. Those, that are furthest from the mirror plane become type-I at $\approx 2\%$ strain as illustrated in Fig. 12.

Stretching the crystal in both x and z directions leads to the mutual annihilation of the neighboring Weyl points and drives the transition from a topological semimetal with eight Weyl points to the trivial semimetal with no Weyl points at all. For the uniaxial y -strain the situation is reversed. Stretching moves the neighboring Weyl points away from each other (2.5% $|G_2|$ for a 2% stretch) and for reasonable strains the number of Weyl points does not change, while compression in this direction leads to annihilation of all points.

We also considered a strain in the $[111]$ -direction, which breaks all the symmetries but time-reversal. The Weyl points survive at small strains, but they move off the high-symmetry $k_z = 0$ plane. This should be expected, since the rotational C_2 symmetry, which in combination with time-reversal allowed the Weyl points to appear on the high-symmetry plane, is now broken, and a stable Weyl point should appear at arbitrary k -points.

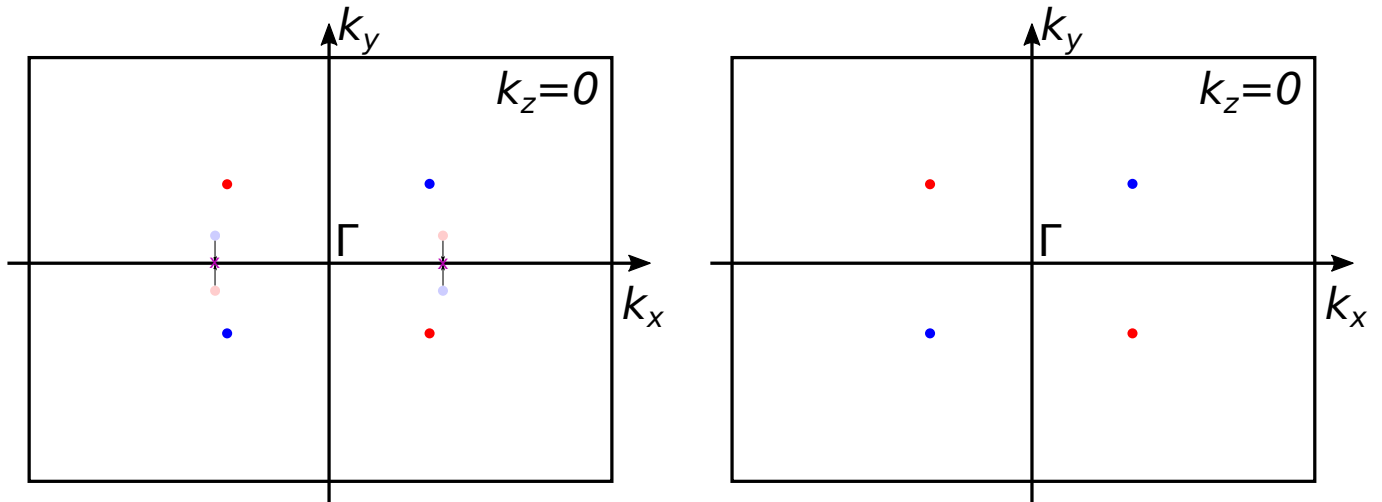


Figure 11: Schematic illustration of the effect of uniaxial compressive strain along the $\hat{x}$ -direction. Left panel: at the strain of $\approx 2\%$ four Weyl points meet in pairs on the mirror plane and annihilate. Right panel: only four Weyl points are left in the $k_z = 0$ plane.

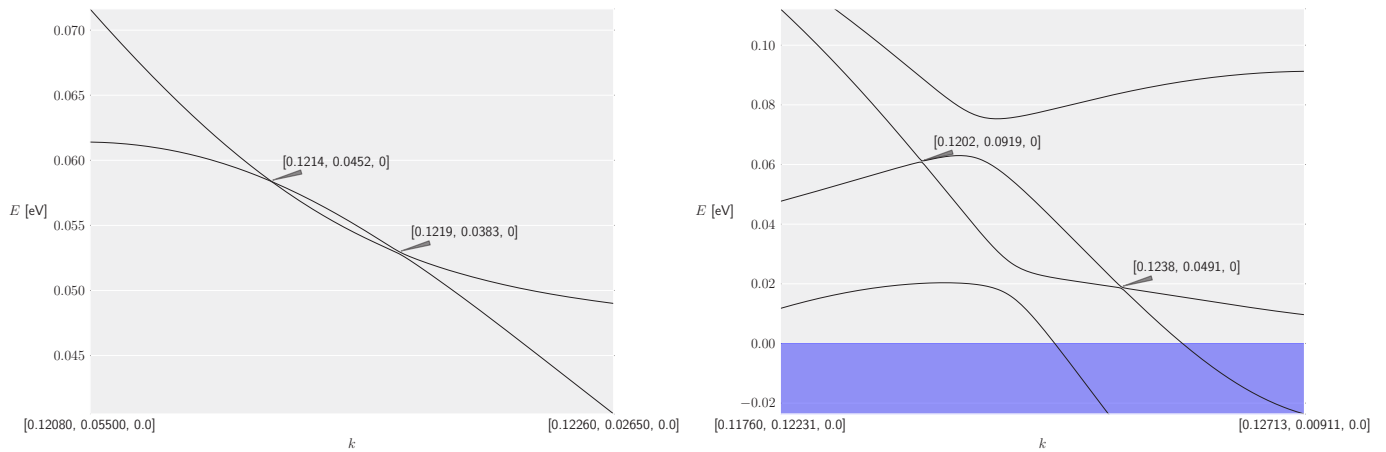


Figure 12: Illustration of type-II to type-I Weyl point transition under the compressive uniaxial strain in the $\hat{z}$ -direction. Left panel: no strain. All points are of type-II. Right panel: 2% strain. The points at higher energy were checked in 3D k -space to be of type-I. The points move further apart in energy, one of them appearing very close to E_F .

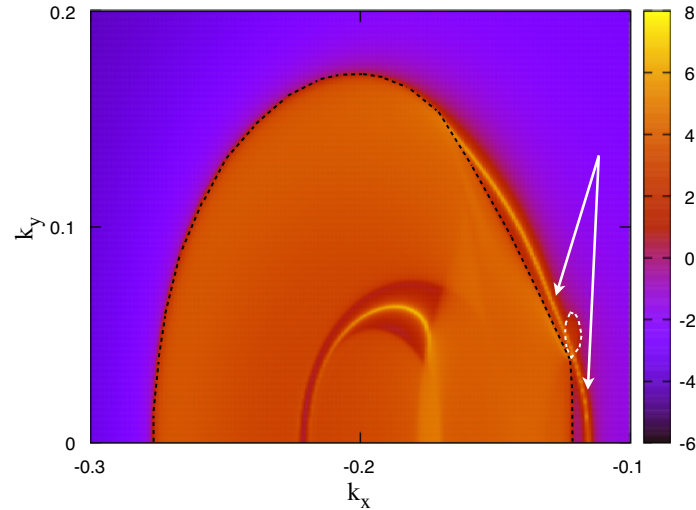


Figure 13: Spectral function illustrates the surface Fermi surface. The surface state, indicated with arrows, emerges in the electron pocket (shown with the black contour), crosses the hole pocket (shown with the white contour), and merges back into the electron pocket (by mirror symmetry).

8 Tight-binding models

To compute chiralities (Chern numbers) of Weyl points, as well as to interpolate between no SOC and full SOC states, tight-binding models were derived with and without SOC. These tight-binding models were obtained using Wannier interpolation [37, 38]. Bloch states were projected onto all W *d*-states and all Te *p*-states. We used a specially symmetrized model without SOC that has the same Weyl points distribution as obtained from first-principles, and interpolated it to the one derived from a fully relativistic calculation.

To get the chiralities of Weyl points for the full SOC case, we used an 88-band tight binding model derived from the full SOC first-principles calculation.

9 Surface states

Here we provide an illustration to support our assertion, made in the main text, about the possibility to move the Fermi arc that crosses the hole pocket into the continuum of the bulk states. Fig. 13 shows a larger scale illustration, where it can be seen that this surface state emerges from the electron pocket and merges back into it. Note that unlike the illustration of Fig. 4(b) of the main text, the small electron pocket becomes part of the larger electron pocket in this illustration. This is due to small deviations ($\approx 10\text{meV}$) of our tight-binding model band structure from its *ab initio* counterpart used for illustrations in Fig. 4 of the main text.

10 Additional Remarks

Matplotlib [41], Mayavi [42] and VESTA [43] software packages were used to create some of the illustrations.

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