The layered transition-metal dichalcogenide WTe$_2$ provides a versatile platform to investigate topologically non-trivial phases [1]. Bulk WTe$_2$ in the $T_d$ phase has been identified as the prototypical example of a Weyl type-II semimetal [2, 3]. In the past few years, particular attention has been paid to the observation of a type-II semimetal [2, 3]. In the past few years, particular attention has been paid to the observation of a type-II semimetal [2, 3]. In the past few years, particular attention has been paid to the observation of a type-II semimetal [2, 3].

We report a detailed Shubnikov-de Haas (SdH) study on the Weyl type-II semimetal WTe$_2$ in magnetic fields up to 29 T. By using the SdH results to guide our density functional theory calculations, we are able to accurately determine its Fermi surface by employing a moderate Hubbard $U$ term, which is an essential step in explaining the unusual electronic properties of this much studied material. In addition to the fundamental orbits, we observe magnetic breakdown, which can consistently be explained within the model of a ‘Russian-doll-nested’ Fermi surface of electron and hole pockets. The onset of magnetic breakdown in WTe$_2$ is solely determined by impurity damping in contrast to magnetic breakdown scenarios in other metallic systems.

The Fermi surface (FS) of bulk WTe$_2$ has been investigated through angle-resolved photoemission spectroscopy (ARPES) [8–15] and quantum oscillation (QO) experiments [10, 14, 16–22]. With previous density functional theory (DFT) band-structure calculations, however, it has proved challenging to correctly explain the size and shape of the small Fermi pockets [4, 8–10, 12, 15–19, 22].

The material has two mirror symmetries and consequently, there are two groups of electron and holes pockets, see Fig. 2(d). The majority of experimental investigations conclude that the FS does indeed comprise two pairs of electronlike pockets and two pairs of holelike pockets, the latter located near the center of the Brillouin zone, sandwiched between the two pairs of electron pockets. Due to the lack of inversion symmetry in WTe$_2$, the spin-orbit interaction leads to a Dreschelhaus spin splitting of the bands and hence the electron and hole FS consist of nested ‘Russian-doll’ pairs [10, 22]. A question remains, however, regarding the exact location of the Fermi level and whether the hole pockets are connected over the $\Gamma$-point forming a ‘dog-bone-shaped’ hole orbit [9, 19] or if additional electron pockets reside in the vicinity of the $\Gamma$-point [13].

One way to solve this long-standing puzzle is to exploit the phenomenon of magnetic breakdown (MB), i.e. tunneling of quasi-particles between distinct (adjacent) pockets of the FS above a threshold magnetic field. This leads to the formation of new orbits consisting of linear combinations of the fundamental frequencies of the associated pockets and thereby constraining further the topology of the FS. Indeed, previous QO studies have shown that MB might occur in WTe$_2$ [10, 13, 21], though a robust identification of these orbits has not yet been done. Additionally, O’Brien et al. proposed that magnetic breakdown in WTe$_2$ occurs between one electron and one hole pocket due to the specific cone structure of a Weyl type-II semimetal whereby electron and hole bands touch each other in $k$-space [23]. Knowing whether this scenario is actually manifested in WTe$_2$ depends on a detailed knowledge of the Fermi surface, which is currently lacking.

In this Letter, we present high-field magneto-transport experiments on a mm-sized WTe$_2$ sample down to $^3$He temperatures. Our analysis of the observed Shubnikov-de Haas (SdH) oscillations, when combined with our DFT calculations determines the precise electronic structure of WTe$_2$ close to the Fermi level. Our subsequent analysis confirms the nested Russian-doll arrangement but suggests that MB can only occur between pockets of the same sign. Moreover, and in contrast with other metallic systems, the onset of MB is found to be solely determined by impurity damping.
WTex flakes were grown by vapor transport method using iodine as the transport agent. Tungsten (99.9%) and tellurium (99.9999%) powders were ground together, pressed to a pellet and pre-reacted in an evacuated silica tube at 750 °C for two days. The product was then reground, pressed into a pellet and loaded into a silica tube with iodine pieces. The tube was placed off-center in a tube furnace to create a temperature gradient of 50 °C between 850 and 800 °C and left to grow for two weeks. Figure 1(a) shows the longitudinal resistance $R_{xx}$ for the sample under study (residual resistance ratio RRR = 30) for various temperatures with the magnetic field $B$ applied along the $c$-axis while the current is passed along the $a$-axis of the sample. For all temperatures, QOs are observed in the FFT spectrum to the extremal areas $A_f$ of the individual pockets: $f = (h/2\pi c)A_f$. Above a threshold magnetic field ($B \geq 8$ T), the QO pattern becomes more complex. In addition to the well-developed low-frequency peaks, a high frequency orbit at 240 T appears (see the [5-28.7][T spectrum in Fig. 2(a)]. This frequency corresponds approximately to the sum of the individual frequencies of the $\alpha$ and $\delta$ orbits, $f_{\alpha+\delta} = f_\alpha + f_\delta$ and is thus a viable signature of MB that will be discussed later.

In Fig. 2(a), fast Fourier Transforms (FFTs) of the $dR_{xx}/dB$ data of Fig. 1(c), are presented for different magnetic field ranges. For the lowest field range [4-10]T, four distinct peaks are observed which we mark as $\alpha$, $\beta$, $\gamma$ and $\delta$ following the labelling of Ref. [16]. For details, we refer to Fig. S1 in the Supplemental Material [25]. Using the Onsager relation, we relate the frequencies $f$ observed in the FFT spectrum to the extremal areas $A_f$ of the individual pockets: $f = (h/2\pi c)A_f$. Above a threshold magnetic field ($B \geq 8$ T), the QO pattern becomes more complex. In addition to the well-developed low-frequency peaks, a high frequency orbit at 240 T appears (see the [5-28.7][T spectrum in Fig. 2(a)]. This frequency corresponds approximately to the sum of the individual frequencies of the $\alpha$ and $\delta$ orbits, $f_{\alpha+\delta} = f_\alpha + f_\delta$ and is thus a viable signature of MB that will be discussed later.

The angle dependence of the SdH oscillations is presented in Fig. 2(b). $B_\perp$ can be determined by maximizing $R_{xx}$ due to the sensitivity of the MR of WTe$_2$ to changes in tilt angle [27]. A commercial Hall probe has been used to extract precise values for the other tilt angles. Both the MR and the QO amplitudes strongly decrease as the sample is rotated from $B_\perp$ (i.e. $B$ parallel to the $c$ axis) to $B_\parallel$ ($B$ parallel to the $a$ axis). In order to map the FS of WTe$_2$, the frequencies of peaks obtained from the FFT spectrum [5-28.7][T multiplied by $\cos \theta$ are plotted as a function of tilt angle $\theta$ in Fig. 2(c) to better visualize.
the quasi-2D nature of the pockets. With increasing \( \theta \), the QO amplitudes of the individual orbits become more and more damped and eventually vanish above 55°. The MB orbit, \( f_{n+4} \) can be observed up to \( \theta = 30° \), as reported previously [16]. The persistence of this orbit over such a wide angular range contrasts markedly with recent observations of MB in nodal-line semimetals [28-30] where the MB orbits are found to vanish exponentially with increasing tilt angles.

To determine the Fermi surface from our extremal orbit size and mass data we use GGA+U DFT calculations [31, 32] with an experimentally determined structure [33]. The calculated Fermi surface is shown in Fig. 2(d) and Fig. 3(c) and consists of two pairs of hole pockets and two pairs of electron pockets which are symmetry distinct. Each pair of electron and hole pockets is nested within each other and the surfaces are symmetrically reflected in the \( \Gamma-Z-Y \) plane. From this Fermi surface we identify the \( \alpha \), and \( \delta \) orbits as originating from the two hole pockets and \( \beta \) and \( \gamma \) from the two electron pockets. Each FS pocket is found to have a single extremal orbit. For such small FS volumes, small shifts in the band-energies are often needed to get perfect agreement with experiment. However, for WTe\(_2\), we find that in addition a moderate \( U \approx 3eV \) must also be employed for the tungsten d orbitals in order to explain the observed value of \( m_e \) for the hole pockets. Without this, the calculated mass is a factor \( \sim 2 \) too high, even after shifting the band energies to match the observed frequencies. Physically, \( U \) models the on-site Coulomb repulsion; an approach which has also been employed for example for the related material MoTe\(_2\) where a similar Hubbard \( U \) value was found [34, 35]. Although the agreement with experiment is not perfect, the residual differences [see Table I and Fig. 2(c)] are acceptably small. Further details of the calculations, including how the results depend on \( U \), are shown in the Supplemental Material [25].

Extraction of the cyclotron masses, \( m_e \), of the individual pockets of the FS is proven to be a challenge for the \( \beta \), \( \gamma \) and \( \delta \) peaks as they are separated by only \( \pm 10 \) T in the FFT spectrum, and a proper range has to be chosen to avoid convolution of their FFT peaks. In Fig. 3(a), the range [5-28.7] T of the FFT spectrum, taken from \( dR_{xx}/dB \), is plotted for different temperatures up to 10 K. Figs. (b), (d), (e), (f) display the FFT amplitudes of the individual peaks as a function of temperature fitted to the temperature-dependent term of the Lifshitz-Kosevich formula, \( R_T = X/\sinh[X] \) with \( X = 2e^2k_BT\hbar/m_eT^2 \), where \( <1/B> = (1/B_{\min})+(1/B_{\max})/2 \). Additional details concerning the mass extraction are discussed in the Supplemental Material [25]. The experimentally extracted cyclotron masses \( m_e \) and those obtained from DFT calculations for each individual pocket are summarized in Table I. In order to separate the FFT peaks a relatively large field range [5-28.7] T is needed, which could in principle lead to an underestimate of the masses. However, the variation in \( m_e \) for the \( \alpha \) pocket on the field range shown in Fig. 3(c), along with additional analysis presented in the Supplemental Material [25] shows this effect is within our errors here.

A further constraint of the FS topology can be made by analysing the MB orbits. Magnetic breakdown occurs if the applied magnetic field \( B > B_0 \approx (h/e)(k_g/2)^2 \), where \( k_g \) is the breakdown gap in \( k \)-space. From our DFT calculations, we extract a gap of \( B_0 = 0.2 \) T for electrons and 0.5 T for holes, respectively. This implies that the Dingle field is around one order of magnitude larger than \( B_0 \), see Supplemental Material [25]. Therefore, MB is determined by impurity damping in WTe\(_2\).
In Fig. 4(a), the FFT spectra obtained from $dR_{xx}/dB$ containing all of the observed MR orbits are shown for several temperatures between 0.34 and 6.5 K in the field range [8-28.7]T. In addition to the $\alpha+\delta$ orbit, we identify four more MB orbits: $\beta+\gamma$, $2\alpha+\delta$, $\alpha+2\delta$, $3\alpha+\delta$. Given our experimental resolution, we are only able to extract the cyclotron masses of the $\alpha+\delta$, $\beta+\gamma$ and $2\alpha+\delta$ orbits, each of which corresponds to the sum of the masses of the individual pockets $[16]$. Their absolute values are summarized in Table II and the corresponding fits are presented in Figs. 4(b)-(d) in which the $R_T$-term has been fitted to the $T$-dependent FFT amplitudes.

![FFT spectra](image)

**TABLE II.** Magnetic breakdown orbits and their extracted cyclotron masses using the field fitting range [8-28.7]T.

| Orbit | $f_0$ (T) | $m_c$ (m_e) | type |
|-------|----------|-------------|------|
| $\alpha+\delta$ | 247 | 1.03 ± 0.04 | hole-hole |
| $\beta+\gamma$ | 283 | 0.79 ± 0.04 | electron-electron |
| $2\alpha+\delta$ | 336 | 1.54 ± 0.19 | hole-hole |

In conclusion, we have performed magneto-transport experiments up to 20 T combined with DFT calculations that enable us to precisely determine the Fermi surface of WTe$_2$. Four individual pockets and their corresponding cyclotron masses have been identified and extracted. The Fermi surface exhibits quasi-2D behavior upon tilting the magnetic field away from the $c$ axis of the crystal. All observed orbits originating from magnetic breakdown have been assigned that further constrains the topology of the Fermi surface. The unprecedented resolution of our high-field study enables us to extract the cyclotron masses of MB orbits and together with the longevity of one of the MB orbits at finite tilt angles, allows for an unambiguous determination of magnetic breakdown in WTe$_2$ that is seen to occur between two electron and hole pockets in a nested Russian-doll configuration.

This work was supported by HFML-RU/NWO-I, a member of the European Magnetic Field Laboratory (EMFL) and by the UK Engineering and Physical Sciences Research Council (Grant No. EP/R011141/1). This publication is part of the project TOPCORE (OCENW.GROOT.2019.048) of the research program NWO - GROOT which is financed by the Dutch Research Council (NWO). We gratefully acknowledge funding from the VILLUM FOUNDATION via the Centre of Excellence for Dirac Materials (11744). M.B. acknowledges the Danish Council for Independent Research, Natural Sciences under the Sapere Aude program (Grant No.702700077B) We thank Malte Rösner and Kamran
Behnia for helpful discussions.

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