Giant anomalous Nernst effect in Weyl semimetals TaP and TaAs

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The discovery of Weyl fermions in transition metal monoarsenides/phosphides without inversion symmetry represents an exceptional breakthrough in modern condensed matter physics. However, exploring the inherent nature of these quasiparticles is experimentally elusive because most of the experimental probes rely on analysing Fermi arc topology or very indirect signatures such as anomalous magnetoresistance. Here we show that the prototypical type-I Weyl semimetals TaP and TaAs possess a giant anomalous Nernst signal with a characteristic saturation plateau beyond a critical field which can be understood as a direct consequence of the finite Berry curvature originating from the Weyl points. Our results thus promote the Nernst coefficient as an ideal bulk probe for detecting and exploring the fingerprints of emergent Weyl physics.

FIG. 1. a) Schematic picture of the Berry curvature originated from right-handed (blue) and left-handed (red) Weyl points. The Weyl points always appear as a pair with opposite chirality separated by $\Delta k$ in the $k$-space and they act as source or sink of Berry curvature (outward or inward arrows). b) Schematic picture of the folding between the energy dependent Fermi distribution function (blue) and entropy density (red) with the diverging Berry curvature (red shaded area) near the Weyl point. The grey shaded area marks the thermal energy $k_B T$. The ANE is particularly large and sensitive to a variation of the chemical potential if the grey and red shaded areas overlap, i. e. $\bar{\mu} \approx k_B T$, which is highlighted in the cases ii) and iii).

Three-dimensional (3D) topological Weyl semimetals (TWSs) [1–7] are characterized by a peculiar electronic structure at half way between a 3D analogue of graphene and topological insulators. Indeed, TWSs present bulk Weyl fermions, chiral particles that disperse linearly along all three momentum directions across the corresponding Weyl points. The Weyl points appear always in pairs, separated in momentum space as consequence of spin-orbit coupling and breaking of the time-reversal symmetry (TRS) or inversion symmetry (IS). Hence, the chiral Weyl fermions experience a finite Berry curvature for which the Weyl points act as source or sink $\mathbf{k}$ (see Fig. 1a). Recently, intrinsic Weyl states have been observed in transition metal monoarsenides/phosphides NbP, NbAs, TaP, TaAs, with naturally broken IS [1–7].

The experimental evidence for the presence of Weyl states essentially concerns the investigation of the topological surface state band structure with the identification of the so-called Fermi arcs. More indirect signatures emerge from magneto-transport measurements, which have recently revealed extremely high carrier mobility $\mu$ [8–10] and negative longitudinal magnetoresistance [11–14] in different candidate materials. These have been indeed interpreted as fingerprints of particles with defined chirality, but unfortunately leave room for ambiguity.

Since a finite Berry curvature at the Fermi level acts on fermions analogous to a magnetic field, the presence of sizeable so-called anomalous transverse transport quantities, viz. the anomalous Hall effect (AHE) and the anomalous Nernst effect (ANE) has been predicted as a more direct, unambiguous proof of a finite Berry curvature and thus the existence of Weyl nodes close to the Fermi level [15, 17–19]. Investigating the Nernst effect is particularly interesting for revealing these sought-after anomalous contributions because in ordinary metals its normal contribution vanishes [20–22], in contrast to the Hall effect, where the normal contribution is always finite and scales reciprocally with the carrier density. In this paper we show that prototypical Weyl semimetals TaP and TaAs indeed possess a giant anomalous component in the Nernst coefficient $S_{xy}$ with a characteristic saturation plateau beyond a critical magnetic field, which univocally certifies these materials as Weyl semimetals in the bulk. We show within a theoretical model that this unique field dependence is the result of a field-induced shift of the chemical potential and a Lifshitz transition due to the separation of the Weyl nodes in momentum space. Our work thus points out the Nernst effect as a smoking-gun experiment for the identification of the emerging Weyl physics in all the candidate materials [7, 21, 27].

We performed thermoelectric measurements in applied magnetic fields on two high quality samples of TaAs and TaP [28]. Fig. 2a shows the magnetic field ($B$) dependence of the Nernst coefficient normalized to the tem-
FIG. 2. The Nernst coefficient data normalized to the temperature, $S_{xy}/T$, of a) TaP and c) TaAs is plotted as a function of $B$. In both of the compounds an anomalous contribution appears as a tendency to saturation. The red dotted lines represent guide for the eyes. The black dashed lines show the results of the phenomenological fit, which well reproduces the experimental data for all the temperatures. Shubnikov-de Haas oscillations appear in the $S_{xy}/T$ vs $B$ curves of TaP at low temperature and they are visible up to 60 K (see Supplementary Information). The Nernst coefficient $S_{xy}$ of b) TaP and d) TaAs is plotted as a function of the temperature $T$. In both of the compounds we find a crossover between two different temperature regimes which appears as a change of slope with a broadened maximum.

temperature, $S_{xy}/T$, for a sample of TaP, in the field range $B = 0 − 14$ T at some selected temperatures. First of all, the absolute value of $S_{xy}/T$ is anomalously large for all the temperatures, overcoming the magnitude of what is typically addressed as ‘giant’ Nernst effect [29]. Remarkably, for $T = 20$ K, 30 K and 50 K, after an initial increase, $S_{xy}/T$ saturates to a constant value for a relatively low $B$, showing an extended plateau for higher fields, superimposed with quantum oscillations. The establishment of flat plateaus represents a strong departure from the conventional theory of transport, which predicts the normal Nernst coefficient $S_{xy}^N$ evolving directly proportional to the magnetic field $B$ or to its inverse $B^{-1}$ in the low and high field limit, respectively [29, 30]. The saturating behavior of $S_{xy}/T$ therefore implies the presence of an anomalous, i.e., a magnetic field independent component in the Nernst signal, which resembles the behavior of ferromagnetic solids [18, 31, 32], but it is strongly unusual in non-magnetic materials.

The inspection of the temperature evolution of the data reveals that such anomalous component dominates the Nernst effect even up to 50 K. However, for $T = 100$ K, even if the tendency of $S_{xy}/T$ to saturate is still persistent, a constant value is not reached (at least for $B < 14$ T) and for $T = 250$ K the curve is almost completely dominated by a linear component, explainable in terms of a normal contribution according to the semi-classical theory. Interestingly, the crossover between a low and a high temperature regime, dominated by an anomalous and a normal contribution respectively, is reproduced in the temperature dependence of $S_{xy}$ for different fields (Fig. 2). In fact, in these curves $S_{xy}$ shows a broadened maximum around 80-100 K for high fields which shifts to lower temperature by decreasing $B$. This maximum exists also in the Nernst coefficient of the analogous compound NbP [34].

In analogy to TaP, we performed Nernst coefficient measurements on a sample of TaAs. Fig. 2 shows the $B$-dependence of $S_{xy}/T$. Unlike the case of TaP, for $T = 20$ K, 30 K and 50 K, the $S_{xy}/T$ vs $B$ curves do not reach a constant value. Even at these low temperatures a $B$-linear component is apparently overimposed to a saturating anomalous part (which is anyway large), leading to a linear drift of $S_{xy}/T$ instead of a plateau for high fields. Remarkably, this normal contribution becomes already dominant around 100 K and it is the only one that persists at 250 K, where the anomalous part is completely unobservable. The difference in the normal component of the Nernst coefficient in the two compounds is not surprising if we consider the strong sensitivity of the conventional Nernst effect even to subtleties of a multi-band electronic structure [29].

We extract the qualitative $T$-dependence of the amplitude of the anomalous part of the Nernst coefficient by using a phenomenological model, which consists of the algebraic sum of the normal $S_{xy}^N$ and the anomalous $S_{xy}^A$ contributions, according to the following equations [33]:

$$S_{xy} = S_{xy}^N + S_{xy}^A,$$

$$S_{xy}^N = S_0^N \frac{\mu_e B}{1 + (\mu_e B)^2},$$

$$S_{xy}^A = S_0^A \tanh(B/B_s),$$

where $\mu_e$ is the average mobility, $S_0^N$ and $S_0^A$ the amplitudes of the normal and the anomalous part, respectively, and $B_s$ the saturation field [33]. The black dashed lines in Fig. 2 and c show the results of the fit of $S_{xy}/T$ for the sample of TaP and TaAs, respectively. The phenomenological model works well for all the temperatures, allowing the isolation of the anomalous component. Fig. 3 shows the $T$-dependence of $S_{xy}^A/T$ for TaP and TaAs. In both the compounds, a jump of around one order of magnitude indicates the transition from a low temperature to a high temperature regime where the anomalous component changes from strong to weak, respectively. The transition starts around 150 K for TaP and 100 K for TaAs. Moreover, it is noteworthy that the transition occurs at the same temperature regime that characterizes a strong change of the Hall resistivity $\rho_{xy}$ which in both compounds results in a very high average Hall mobility at low temperatures [8, 10, 37]. This high mobility has been attributed to the suppression of back-scattering due to the emergence of Weyl fermions [8, 10].
to a finite $\Omega^z_n (k)$ and $f_{n,k}$ (or $s_{n,k}$) which becomes particularly strong when $\mu$ moves towards the Weyl point. [?] The ANE therefore becomes sensitive to both, variations of the chemical potential $\mu$ and of the temperature $T$. More specifically, it is expected to grow upon reducing the chemical potential as well upon increasing the temperature from $k_B T \ll \tilde{\mu}$ toward $k_B T \approx \tilde{\mu}$, where $\tilde{\mu}$ measures the distance between the Weyl node and the chemical potential.

**Magnetic field-induced shift of the chemical potential**

If a magnetic field is applied to a Dirac or Weyl semimetal with the Dirac or Weyl points in the vicinity of the chemical potential, the latter typically experiences a field-induced shift. This can be inferred from Fig. 4 where for simplicity the effect of a magnetic field applied on a doubly degenerate Dirac cone along the $z$-direction is considered. We start with the zero-field case $B = 0$. Here, the $k_z$-dispersion around a Dirac point is schematically represented by the red solid line in Fig. 4. The chemical potential $\mu$ takes a certain position (red dotted horizontal line) above the node, determined by the number of conducting electrons, which corresponds at zero-temperature to the number of the occupied states below the Fermi level. The application of a magnetic field along the $z$-direction splits the Dirac cone into two Weyl cones which immediately leads to a finite ANE. The magnitude of this ANE remains small as long as $k_B T \ll \tilde{\mu}$ (cf. situation i) in Fig. 4. Increasing the magnetic field, however, leads to a further separation of the Weyl nodes (blue solid lines) where the inevitable downshift of unoccupied states causes a reduction of the chemical potential $\mu$ in order to fulfill the condition of a fixed particle number. Thus, the distance between the Weyl points and the chemical potential, $\tilde{\mu}$, is reduced resulting, as discussed above, in an enhancement of the ANE, in agreement with the experiment. For larger fields, $\mu$ is pushed to the region where the Weyl cones are separated, such that the Fermi surface topology has changed. This regime is sketched in Fig. 4 by orange and green lines. Here, $\mu$ has approached the separated Weyl nodes and two separated Fermi surfaces appear. In contrast to the behavior at low fields as explained above, in this regime the chemical potential remains nearly constant since a further increasing magnetic field simply leads to further separation of the Weyl nodes but not to a change of the dispersion near the Weyl nodes. As we will discuss in detail below, this mechanism works also if the starting situation at $B=0$ is not a degenerate Dirac cone but two preformed Weyl nodes, as in case of inversion symmetry breaking TWS, since the driving parameter is the additional shift in momentum space induced by the field and the consequent variation of the $k$-space volume.

This behavior qualitatively explains the observed saturation of the Nernst coefficient when the magnetic field is larger than some material characteristic value $B_s$ as

$$\sigma^{\chi}_{xy} = \frac{e^2}{\hbar} \sum_n \int \frac{d^3k}{(2\pi)^3} \Omega^z_n (k) f_{n,k}$$

$$\alpha^{\chi}_{xy} = \frac{e^2}{\hbar} \sum_n \int \frac{d^3k}{(2\pi)^3} \Omega^z_n (k) s_{n,k}.$$
schematically presented in Fig. 4.

In the case of a Weyl semimetal, the value of $B_s$ can readily be estimated in the frame of the above scenario. To this end, we have numerically evaluated $\mu$ as a function of $B$ based on the minimal dispersion model for Weyl fermions given by $E_k = \pm \sqrt{v_F^2(k_x^2 + k_y^2) + (gB \pm v_F k_z)^2}$ [15]. We obtained the following relation between $B_s$, the total Fermi volume in zero field, $\Delta V = \int d^3k f(k, \mu)$ and the Fermi velocity $v_F$: \[ B_s = v_F \frac{m_e}{e} \sqrt{\frac{3\Delta V}{2\pi}} \cdot 0.745, \tag{6} \]

where $m_e$ denotes the electron mass and $e$ the elementary charge. The number 0.745 in Eq. (6) corresponds to the ratio of the saturated value of the chemical potential compared to its original value, $\mu_s/\mu = 0.745$, where both $\mu_s$ and $\mu$ are related to the energy of the Weyl point. For Weyl semimetals such as TaP and TaAs, $\mu_s/\mu$ assumes a material specific different value. From band structure calculations [35] one finds for these materials preformed Weyl points along $k_x$ (with a relative distance $\Delta k_x$ of the order of $10^{-2}$ Å$^{-1}$ in the $k$-space). The anomalous $S_{xy}$ measured here has been observed with the magnetic field applied in the $z$-direction, inducing a further separation of the Weyl nodes along $k_z$, where for both TaAs and TaP $\Delta k_z = 2gB/v_F$ ($g$ is the Lande factor) is of the order of $4 \cdot 10^{-3}$ Å$^{-1}$ at $B = 10$ T. Band structure calculations show that in both materials there are two relevant pairs of Weyl points, usually denoted as $W_1$ and $W_2$, which are close to the Fermi level and thus contribute to the anomalous transport. To obtain our saturation effect at least one pair needs to be enclosed by a non-separated Fermi surface. Upon closer inspecting the band structure results [35] one finds that in TaP $W_2$ has a separated Fermi surface. However, for $W_2$ the saddle point between the pair of Weyl points is roughly 0.015 eV below the Fermi level (Weyl point energy: -0.05 eV) indicating a non-separated Fermi surface in zero-field. This property allows to obtain the discussed saturation effect through a shift of the chemical potential at moderate field values. In the specific situation of TaP the above numbers suggest a somewhat enhanced $\mu_s/\mu = 0.751$ and thus, following Eq. (6), $B_s = 3.3$ T, where $\Delta V \approx 10^{-9}$ Å$^{-3}$ and $v_F \approx 10^5$ m/s have been used as approximate values [35]. For TaAs, on the other hand, for both Weyl points the Fermi surface is already separated according to band structure calculations. Nevertheless, the described saturation effect is observed also in this material. We attribute this materials specific discrepancy between the experiment and the quantitative predictions to shortcomings of the precision of band structure calculations. Note that the saddle point energy of $W_1$ in TaAs is calculated to a value of approximately 0.01 eV which is slightly above the Fermi level. However, a precise description of one-particle states at such small energy leading to the typical small Fermi volumes in Weyl semimetals requires an exceptional high $k$ point sampling in the band structure calculation. Therefore, we believe that an improvement in such a direction could lead to a correction of the saddle point energy leading to a situation similar to TaP.

Impact of temperature Due to the broadening of $f_{n,k}$ (or $s_{n,k}$) a variation of the temperature instead of $\mu$ should also affect the ANE [25]. This effect predicts at low temperature an enhancement of the ANE with increasing temperature. The increase is expected to continue upon raising the temperature until close to $k_B T \approx \tilde{\mu}$, where the thermal occupation of the Weyl states at energies above and below the Weyl node is practically the same, resulting in a strong reduction of the ANE. Note, however, that at very large temperature and also in the case where the Weyl point is placed exactly at the Fermi level corrections to the Boltzmann theory are necessary. Remarkably, both the low-temperature increase and the high-temperature crossover towards smaller values are observed in our experimental results (Inset of Fig. 3). Note that the high-temperature reduction of the ANE in TaP occurs at higher temperature with respect to the case of TaAs. This is consistent with band structure calculations which yield an about a factor of two larger energetic position $\tilde{\mu}$ of the lowest lying Weyl point in TaP as compared to TaAs. Note that the Weyl points at positive energy can also contribute to the anomalous transport at high temperature but the same arguments for the reduction of the ANE are also valid there.

In conclusion, we reported the observation of a giant ANE in the two Weyl semimetals TaAs and TaP. The occurrence of this ANE can be understood as a direct evidence for a large Berry curvature and thus the Weyl points close to the Fermi level, which qualifies Nernst effect measurements as a valuable tool to elucidate Weyl physics. We have shown that the unique identifying feature of the ANE, viz. the occurrence of field independence beyond a critical field can be traced back to a strong sensitivity of the ANE to field-induced changes of the chemical potential and a Lifshitz transition due to the separation of the Weyl points in momentum space.

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FIG. 4. Schematic behavior of the chemical potential in a Weyl semimetal. In zero-field (red line) the energy dispersion shows only one single Dirac node which is placed in the Γ-point. Application of magnetic field leads to the appearance of two nodes (blue solid line) which are separated in momentum space proportional to the magnetic field. The expected shift of the chemical potential \( \mu \) under variation of the magnetic field is indicated by the dotted lines. a) Schematic change of the dispersion from \( B = 0 \) (red solid line) to a relatively small value \( B_1 < B_2 \) (blue solid line) where \( B_2 \) is a representative field value where the saturation of the Nernst coefficient sets in. The change of \( \mu \) (downshift from the red to the blue dotted line) is responsible for the observed strong variation of the Nernst coefficient below \( B_1 \) (blue solid line) where \( B_2 \) (red solid line) is already achieved under variation of the magnetic field and the occurrence of two separated Fermi surfaces the conservation of the particle number (area between the dashed lines) is already achieved if the chemical potential remains almost fixed. As a consequence, the anomalous Nernst coefficient \( S_{\text{an}}^y \) will also not change as highlighted in panel c).

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