Physics 180C: Quantum Oscillations in the Resistivity of TaAs

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(Dated: March 21, 2020)

We study the three-dimensional transition-metal pnictide material TaAs using quantum oscillations in the longitudinal resistivity (Shubnikov–de Haas effect) at temperatures ranging from 2.2 K to 10 K. We show that (1) TaAs exhibits a negative magnetoresistance (chiral anomaly) consistent with the presence of Weyl nodes near the Fermi level, (2) the effective mass varies linearly with the applied field, consistent with a linear dispersion at the Fermi energy and a degeneracy lifted through Zeeman splitting, and (3) the geometric phase accumulated by electrons during cyclotron orbits is $\gamma = (0.910 \pm 0.043)\pi$, indicating the presence of Weyl nodes. We conclude that TaAs is a Weyl semimetal.

INTRODUCTION

Fermions obey the Dirac Equation:

$$(i\gamma^\mu \partial_\mu - m)\Psi = 0 \tag{1}$$

The γ^μ are 4-matrices, and we can define the chiral projection operators:

$$L \equiv \tfrac{1}{2}(1 - i\gamma^0\gamma^1\gamma^2\gamma^3) \tag{2}$$
$$R \equiv \tfrac{1}{2}(1 + i\gamma^0\gamma^1\gamma^2\gamma^3) \tag{3}$$

So that the Fermion field can be written as a combination of its "left handed" and "right handed" components:

$$\Psi = L\Psi + R\Psi \tag{4}$$

Setting the mass to zero decouples the Dirac equation into left handed and right handed solutions. It so happens that these solutions, known as Weyl fermions, are irreps of the Lorentz group and so can be used to construct any Fermion field.

Semimetals are compounds in which multiple bands cross the Fermi surface. A possible semimetal of interest is one with intersecting bands at the Fermi surface, and a linear dispersion relation at the Fermi surface demonstrating Fermi arcs. Such a material would host Weyl fermions at these intersections or Weyl nodes.

In 2015, a number of groups reported ARPES measurements of the electronic structure of TaAs that proved it is a Weyl semimetal [1–3]. Soon thereafter, studies of quantum oscillations in TaAs bolstered this result [4, 5].

We reproduce these results with the Shubnikov de Haas Effect (quantum oscillations in longitudinal resistance) by showing that: (1) TaAs exhibits a negative magnetoresistance consistent with the presence of Weyl nodes near the Fermi level, (2) the effective mass varies linearly with the applied field, consistent with a linear dispersion at the Fermi energy, and (3) the geometric phase accumulated by electrons during cyclotron orbits is $\gamma = (0.910 \pm 0.043)\pi$.

Effective Mass and Cyclotron Motion

In a solid, electrons respond to applied forces with an effective mass, m^* such that:

$$F = m^* a \tag{5}$$

Therefore, electrons can be treated as free with an effective mass, instead of as experiencing a potential:

$$E = \frac{p^2}{2m^*} \tag{6}$$

Which directly leads to:

$$\frac{1}{m^*} = \frac{\partial^2 E}{\partial^2 p} \tag{7}$$

Where momentum is given by the de Broglie relation:

$$p = \hbar k \tag{8}$$

An electron in free space subject to a constant perpendicular magnetic field of strength B, will orbit in circles. Representing this in the Hamiltonian formalism in the Landau gauge:

$$H = \frac{1}{2m_e}[p_x^2 + (p_y + eBx)^2] \tag{9}$$

Whose spectrum is Landau Levels for integers $n > 0$:

$$E_n = \hbar\omega_c \left(n + \tfrac{1}{2}\right) \tag{10}$$

Where ω_c is the cyclotron frequency of the oscillations:

$$\omega_c = \frac{eB}{m_e} \tag{11}$$

This means the frequency in a solid for constant α is:

$$\omega_c^* = \frac{eB}{m^*} = \frac{eB}{\alpha m_e} \tag{12}$$

Shubnikov de Haas Effect

Now we note that the electronic density of states is high near the Landau Level center and low between Landau Levels. Additionally, the Landau Level spacing is inversely dependent on the magnetic field, so the density of states at the Fermi energy will oscillate periodically in $1/B$ as the applied magnetic field is varied.

Quantities including the resistance depend on the density of states at the Fermi energy, and the oscillations in the resistance for varied applied magnetic field are known as the Shubnikov de Haas Effect.

In particular, we will be interested in the longitudinal resistivity, whose oscillations are observed in $\Delta\rho_{xx}$:

$$\Delta\rho_{xx}(B,T) = \rho_{xx}(B,T) - \rho_{xx}(B,T_{\text{high}}) \tag{13}$$

Usually, $\Delta\rho_{xx}(B,T) > 0$, however in Weyl semimetals, $\Delta\rho_{xx}$ can become negative, indicating the chiral anomaly of the Weyl nodes.

Lifshitz-Kosevich Formalism

These quantum oscillations will be attenuated by environmental factors. We address this using the Lifshitz-Kosevich formalism, which relates attenuation factors arising from finite temperature, impurity scattering and spin-splitting through the formula [7]:

$$\Delta\rho_{xx} \propto R_T R_D R_S \tag{14}$$

The expressions in a three dimensional metal yield:

$$\Delta\rho_{xx} \propto \frac{2\pi^2 kT/\hbar\omega_c^*}{\sinh(2\pi^2 kT/\hbar\omega_c^*)} \exp\left(-\frac{\pi m_b}{eB\tau}\right) \cos\left(\frac{\pi g m_s}{2m_e}\right) \tag{15}$$

With temperature independent R_D and R_S, and substituting for ω_c^* (in SI units):

$$\Delta\rho_{xx}(B,T) \propto \frac{14.6932\,\alpha\ T/B}{\sinh(14.6932\,\alpha\ T/B)} \tag{16}$$

For fixed B and varying T, the effective mass $m^* = \alpha m_e$ may be interpolated.

At a Weyl node, the dispersion is linear, and so the effective mass goes to zero. As the degeneracy at the node is lifted through an applied magnetic field in Zeeman splitting, the effective mass increases linearly.

Geometric Phase

In the absence of environmental coupling, the wavefunction as dependent on time is the initial wavefunction propagated by the dynamic evolution operator and the geometric evolution operator, represented here by their eigenvalues, $\theta(t)$ and $\gamma(t)$, respectively:

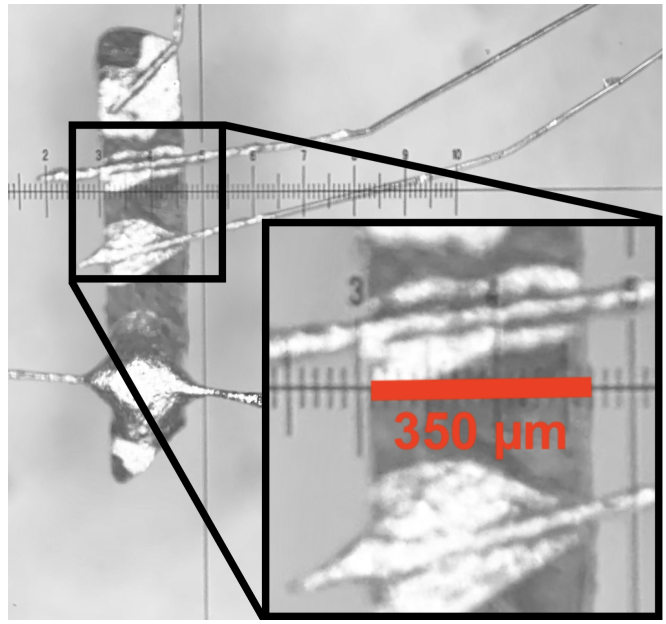

FIG. 1. A sample as photographed under optical microscope. Insert emphasizes the dimensions of the conducting region. Sample dimensions between the inner leads are: length = 355±21 μm, width = 351±5 μm, and depth = 50±6 μm. This sample did not produce oscillations, so we analyzed another group's data, and considered oscillations of resistance rather than resistivity since the sample dimensions were unknown.

$$\psi(t) = \psi(0)e^{i\theta(t)}e^{i\gamma(t)} \tag{17}$$

The dynamic phase factor is:

$$\theta(t) = -\frac{1}{\hbar}\int_0^t d\bar{t}E(\bar{t}) \tag{18}$$

The geometric phase factor about a path P is:

$$\gamma(P) = i\oint_P \langle\psi(\boldsymbol{r})|\nabla_{\boldsymbol{r}}|\psi(\boldsymbol{r})\rangle \cdot d\boldsymbol{r} \tag{19}$$

Here we are interested in the path traversed by an electron in one cyclotron orbit. In a normal metal the geometric phase will be 0, while if a Weyl node is enclosed in the cyclotron orbit, the geometric phase will be π. [6]

The Lifshitz-Onsager quantization rule gives:

$$\frac{\hbar A_n}{eB} = 2\pi n + (1+2\delta)\pi - \gamma \tag{20}$$

So, for oscillation frequency f, and constant δ we have:

$$\Delta\rho_{xx}(B,T) = A(B,T)\cos(2\pi f/B + [(1+2\delta)\pi - \gamma]) \tag{21}$$

EXPERIMENTAL METHODS

We were given a TaAs single crystal by the Ni research group. We then prepared the sample by using fine sand paper to remove the oxide layer on the sample. Next, we connected four wires to the sample using conductive silver glue. We then measured sample dimensions. Next we soldered the wires to the four-wire voltage electrodes of a DC measurement puck. Note that we need to use a four-wire measurement since we use small currents and we expect the resistivity of our sample to be low, and voltages can be more accurately measured than currents.

We then applied magnetic fields perpendicular to the sample (and presumably the crystal lattice) in steps of roughly 0.009 T from 9 T to −9 T at temperatures of 2.2, 3.0, 4.0, 6.0, 8.0, and 10.0 K using a Quantum Design DynaCool Physical Property Measurement System and measured the resistance using a four-wire resistance measurement.

ANALYSIS AND RESULTS

We begin by processing the measured data Fig. 2 by subtracting the high-temperature-behavior background as in Eqn. 13 and noting that the longitudinal resistance is even under inversion of the magnetic field, while the transverse resistance is odd under inversion of the magnetic field. A function $f(x)$ may be written as the sum of an even function and an odd function:

$$f(x) = \underbrace{\tfrac{1}{2}(f(x)+f(-x))}_{\text{even}} + \underbrace{\tfrac{1}{2}(f(x)-f(-x))}_{\text{odd}} \qquad (22)$$

This yields the Shubnikov de Haas oscillations as shown in Fig. 2. Considering these at each of the temperatures and plotting the resistance against the inverse field shows oscillations periodic in $1/B$ as in Fig. 3, as illustrated by the Fourier transform of the oscillations in Fig. 3.

A fit of the temperature-dependent amplitudes at the main pocket using the Lifshitz-Kosevich formalism as in Eqn. 16 yields the effective mass as shown in Fig. 4. Evaluating this for the other peaks shows that the effective mass is linear in the applied field as shown in Fig. 4.

Additionally, the geometric phase γ arises in the product of the linear function $A(T, B)$ with a modulating cosine as in Eqn. 21. If we take one point per cycle at the same phase of a linear function modulated by a periodic function and plot the points versus the oscillation index, the point of intersection with the x-axis, x, gives the phase (mod 2π), which enables us to calculate the geometric phase as shown in Fig. 5. Mathematically:

$$2\pi x = (1+2\delta)\pi - \gamma \quad \Leftrightarrow \quad \gamma = [1+2(\delta - x)]\pi \qquad (23)$$

Results

We observe that TaAs exhibits a negative magnetoresistance at some values of the applied field consistent with the presence of Weyl nodes near the Fermi level. Additionally, the effective mass varies linearly with the applied field, as $m^*/m_e = (0.04401 \pm 0.00036)B$, consistent with a linear dispersion at the Fermi energy and a degeneracy lifted through Zeeman splitting. Finally, we find that the geometric phase accumulated by electrons during cyclotron orbits is $\gamma = (0.910 \pm 0.043)\pi$, indicating the presence of Weyl nodes.

We believe that the dominant source of error in our measurements was the alignment of the crystal with the magnetic field which produces a systematic error.

CONCLUSION

We observed quantum oscillations in the longitudinal resistivity of a TaAs single crystal subject to an applied magnetic field. We observed the amplitudes were sometimes negative which indicates a chiral anomaly. Additionally, we analyzed the oscillations and found that the effective mass varied linearly with the applied field, and that the geometric phase accumulated by electrons during a cyclotron orbit agreed with π. These observations support the hypothesis that TaAs is a Weyl semimetal.

If we were to repeat the experiment, we would have liked to test more samples and explore their behavior in higher fields at more temperatures (colder and warmer). It would also be interesting to vary crystal orientation and map the Fermi surface.

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[1] B. Lv, H. Weng, B. Fu, X. Wang, H. Miao, J. Ma, P. Richard, X. Huang, L. Zhao, G. Chen, *et al.*, Phys. Rev. X **5**, 031013 (2015).

[2] S.-Y. Xu, I. Belopolski, N. Alidoust, M. Neupane, G. Bian, C. Zhang, R. Sankar, G. Chang, Z. Yuan, C.-C. Lee, *et al.*, Science **349**, 613 (2015).

[3] L. Yang, Z. Liu, Y. Sun, H. Peng, H. Yang, T. Zhang, B. Zhou, Y. Zhang, Y. Guo, M. Rahn, *et al.*, Nat. Phys. **11**, 728 (2015).

[4] X. Huang, L. Zhao, Y. Long, P. Wang, D. Chen, Z. Yang, H. Liang, M. Xue, H. Weng, Z. Fang, *et al.*, Phys. Rev. X **5**, 031023 (2015).

[5] F. Arnold, M. Naumann, S.-C. Wu, Y. Sun, M. Schmidt, H. Borrmann, C. Felser, B. Yan, and E. Hassinger, Phys. Rev. Lett **117**, 146401 (2016).

[6] N. Armitage, E. Mele, and A. Vishwanath, Rev. Mod. Phys. **90**, 015001 (2018).

[7] I. Lifshitz and A. Kosevich, Sov. Phys. JETP **2**, 636 (1956).

[8] H. Murakawa, M. Bahramy, M. Tokunaga, Y. Kohama, C. Bell, Y. Kaneko, N. Nagaosa, H. Hwang, and Y. Tokura, Science **342**, 1490 (2013).

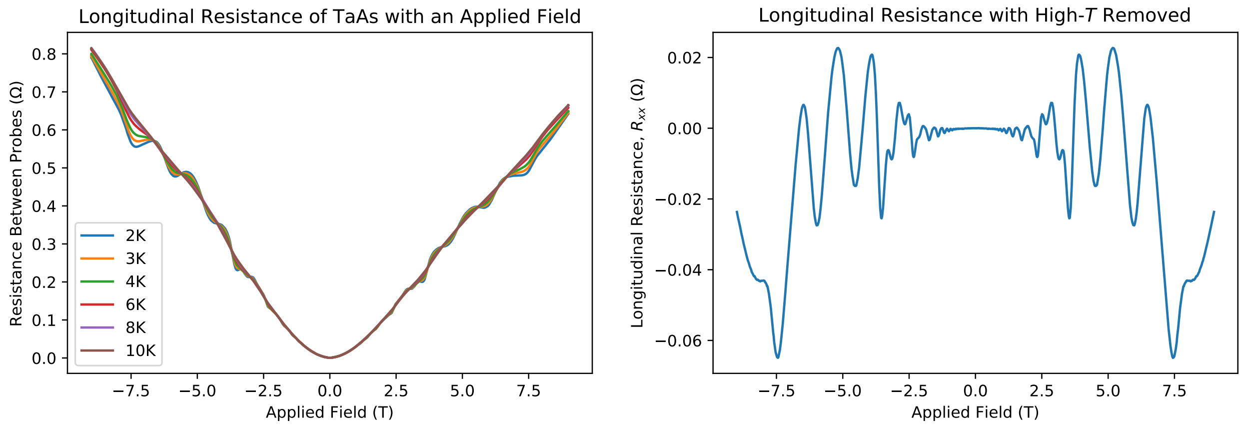

FIG. 2. (left) Measured longitudinal resistivity at a variety of temperatures. Oscillations are of larger amplitude at lower temperatures. Plot is not an even function due to imperfections in the electrode alignment and angle of the sample with respect to the applied field. (right) Oscillations in the measured 2.2 K data extracted through (1) subtracting high temperature behavior (10 K data), and (2) made even to remove the transverse resistance and account for potential alignment issues. We observe negative longitudinal resistance at many fields, which corresponds to a chiral anomaly and is consistent with the presence of Weyl nodes near the Fermi energy.

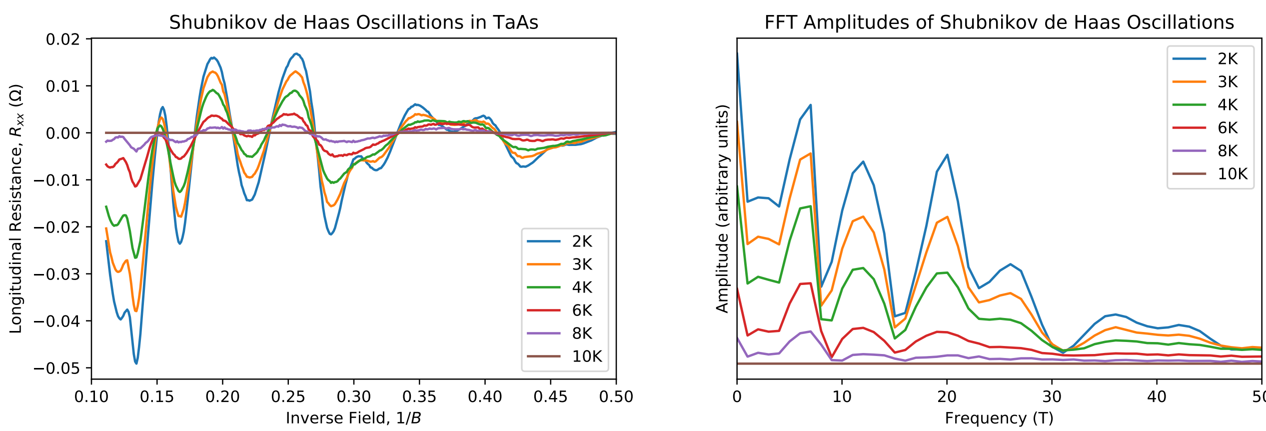

FIG. 3. (left) Shubnikov de Haas oscillations in the longitudinal resistivity of TaAs sample at temperatures from 2.2 to 10 K. (right) Fourier decomposition of resistivity oscillations. We observe peaks at frequencies near 7, 12, and 20 T.

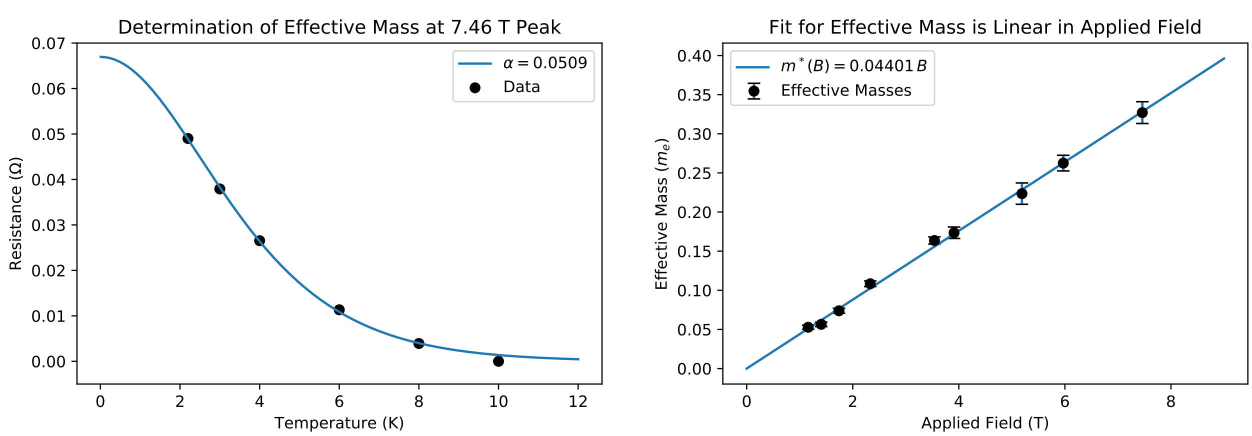

FIG. 4. (left) Determination of the effective mass at the 7.46 T peak by fitting the thermal attenuation term of the Lifshitz-Kosevich formula to the temperature dependence of the peak amplitude. We find the effective mass is $m^* = (0.0509 \pm 0.0011)m_e$. (right) Effective masses determined at each extrema of the resistivity oscillations using the Lifshitz-Kosevich formalism. We observe that the measured effective masses vary linearly with the applied field. We explain this by supposing there exists a Weyl node at the surface at zero field whose degeneracy is lifted by the applied magnetic field.

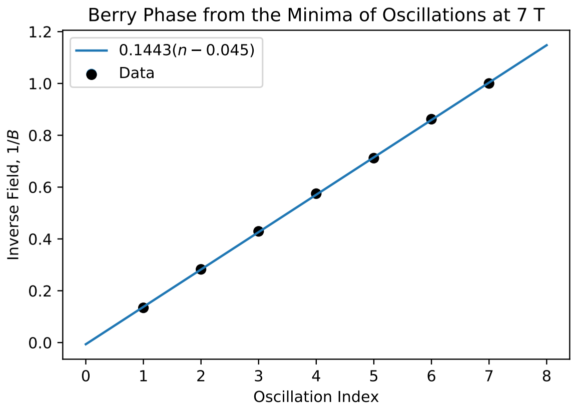

FIG. 5. The magnetic field values corresponding to the low frequency minima are plotted with indices (integer offset from the Landau Level index) to give the phase offset in the interval $[0, 2\pi]$. We observe the x-intercept is at 0.045 ± 0.022, corresponding to a geometric phase of $\gamma = (0.91 \pm 0.043)\pi$ in the two dimensional limit of $\delta = 0$ [8]. Uncertainties are on the order of the marker size.