ROLE OF SPIN-ORBIT COUPLING AND EVOLUTION OF THE ELCTRONIC STRUCTURE OF WTE_2 UNDER AN EXTERNAL MAGNETIC FIELD

D. Rhodes[1,2], S. Das[1,2], Q. R. Zhang[1,2], B. Zeng[1], N. R. Pradhan[1], N. Kikugawa[3,1], E. Manousakis[1,2,4], and L. Balicas[1]

[1]*National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, USA*
[2]*Department of Physics, Florida State University, Tallahassee, Florida 32310, USA*
[3]*National Institute for Materials Science, Tsukuba, Ibaraki 305-0047, Japan*
[4]*Department of Physics, University of Athens, Panepistimioupolis, Zografos, 157 84 Athens, Greece*

Here, we present a detailed study on the temperature and angular dependence of the Shubnikov–de Haas (SdH) effect in the semimetal WTe_2. This compound was recently shown to display a very large non-saturating magnetoresistance which was attributed to nearly perfectly compensated densities of electrons and holes.[1] We observe four fundamental SdH frequencies and attribute them to spin-orbit split, electron-like, and hole-like Fermi-surface (FS) cross-sectional areas. Their angular dependence seems consistent with ellipsoidal FSs with volumes suggesting a modest excess in the density of electrons with respect to that of the holes, shown in figure 1.

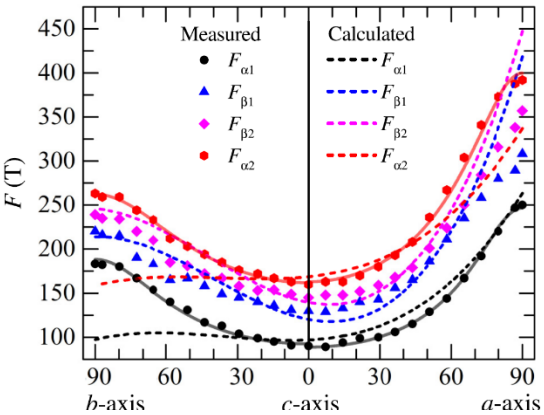

Figure 1: Position of the main four peaks detected in fast Fourier spectra as a function of the orientation of the field relative to the crystallographic axes. Dashed lines depict the DFT-calculated angular dependence of the frequencies. Solid lines correspond to fits assuming ellipsoidal Fermi surfaces.

We show that density functional theory (DFT) calculations fail to correctly describe the FSs of WTe_2.When their cross-sectional areas are adjusted to reflect the experimental data, the resulting volumes of the electron/hole FSs obtained from the DFT calculations would imply a pronounced imbalance between the densities of electrons and holes. We find evidence for field-dependent Fermi-surface cross-sectional areas by fitting the oscillatory component superimposed onto the magnetoresistivity signal to several Lifshitz-Kosevich components. We also observe a pronounced field-induced renormalization of the effective masses.

Taken together, our observations suggest that the electronic structure of WTe_2 is nearly, but not perfectly compensated and evolves with the magnetic field due to the Zeeman splitting. This evolution is likely to contribute to its pronounced magnetoresistivity.

[1] M. N. Ali, *et al.*, Nature (London) **514**, 205 (2014).

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Email: Rhodes@magnet.fsu.edu
Balicas@magnet.fsu.edu