Modeling Fermi Surfaces in Topological Materials

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While at the University of Michigan, I utilized the programs Origin and Wien2k to compare torque magnetometry experimental data and density functional theory (DFT) calculations based on open-source information. By modeling the fermi surface and band structures of these materials, we are able to understand how best to exploit their non-trivial topological properties.

Background

Topological materials are those that display non-trivial topological effects. They are characterized by strong spin-orbit locking and time reversal symmetry. Because their topology makes for such great conducting surfaces, they are of interest to the scientific community for applications such as topological quantum computing.

Torque Magnetometry

Thus, it is imperative that we understand topological materials' electronic structures. One of the ways to gain useful information is through torque magnetometry. Torque magnetometry probes the material by applying a magnetic field at varying temperatures or angles. By applying a magnetic field, one may observe the following two phenomena: the de Haas-van Alphen (dHvA) and Shubnikov-de Hass (SdH) effects. For these effects, a change in applied magnetic field causes quantum oscillations which change magnetic susceptibility in the case of dHvA and a change in conductivity in the case of SdH. For the purposes of this study, I focused on the dHvA effect. While one cannot directly see quantum oscillations, their effects may be measured via their impacts.

The relationship between magnetic susceptibility and magnetic moment may be described by the following equation:

$$\chi_m = \frac{N_A \mu_0}{3k \cdot T} \mu^2 \quad (1)$$

Where χ_m is the magnetic susceptibility, T is temperature, k is Boltzmann's constant, μ_0 is the permittivity of free space, N_A is Avogadro's number, and μ is the magnetic moment. So from this, by changing the applied magnetic field, the magnetic moment is thus changed. And,

$$\tau = \mu \times B \quad (2)$$

Thus, by changing the applied field, the moment changes, causing a torque. This is the theory behind Professor Li's torque magnetometry method. A device (Fig. 1) was created such that a magnetic torque would cause a change in the position of the sample. By changing the sample position, the space between the sample and the lower Au film would cause a measurable change in capacitance as per the following equation:

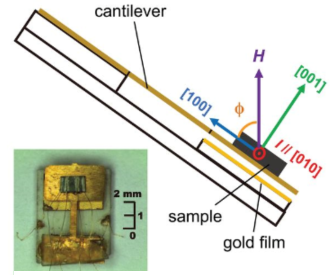

Figure 1-Torque magnetometry setup [1]

$$C = \varepsilon\left(\frac{A}{d}\right) \tag{3}$$

Where C is capacitance, ε is the absolute permittivity, A is the area of the capacitor (which remains constant), and d is the distance between the 2 electrodes of the capacitor. Thus, there is now a measurable quantity to observe quantum oscillations.

The data is received in the quantity of magnetic moment. Using origin, the background may be subtracted, allowing us to see the magnetic moment as a function of the applied field (H) over varying temperatures. Li lab has the capability of reaching extreme conditions (20mK, 14T) allowing a clear visual of the impacts of the field. An example of what this looks like is seen in Fig. 2.

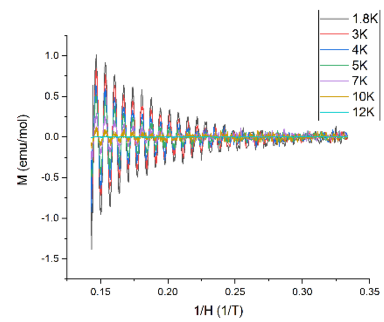

Figure 2-oscillation of magnetic moment of Hf_2Te_2P as a function of the reciprocal

From here, an FFT analysis is run to observe the band frequencies involved in this phenomenon. The peaks seen reflect the band frequencies in the units of tesla. For this material, Hf_2Te_2P, the band frequencies are approximately 147 and 110 T.

Then, by observing frequency peak amplitude as a function of temperature, the Dingle temperature may be found. This is not a physical temperature, rather a means of deriving the Berry phase of the material and the effective mass of the charge carriers. After deriving these properties, they are used alongside the following equation to create a model predicting the magnetic moment arising from an applied field. The equation is as follows:

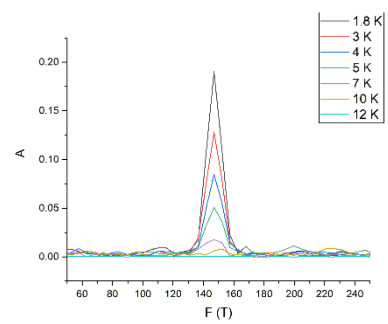

Figure 3-FFT of magnetometry data

$$M\alpha\left(\frac{B}{|\partial^2 a_F/\partial_k^2|}\right)^{1/2}\sum_{r=1}^{\infty}\frac{(-1)^r}{r^{3/2}}R_D R_T R_s \sin[2\pi r\left(\frac{F}{B}-\gamma\right)\pm\frac{\pi}{4}] \tag{4}$$

Where *M* is the magnetic moment, *B* is the applied field, *r* will be 1 in this case, *F* is the frequency, and γ is related to the Berry phase. The different *R*'s are related to different influences on the resulting moment. Making frequency, Dingle temperature (embedded in R_D), effective mass (embedded in each R term) and phase shift parameters of the equation, Origin was able to derive these quantities to confirm what was previously calculated. These indeed matched, providing a corresponding graph as what was experimentally found. The reason for these measurements is to provide an indication of the presence of a Dirac band, characteristic with its small effective mass and non-trivial Berry phase. The found effective masses were 0.27 for 110 T and 0.22 for 147T which also had a Berry phase of 0.64, thus as both conditions are met, further knowledge is desired in terms of the Fermi surface.

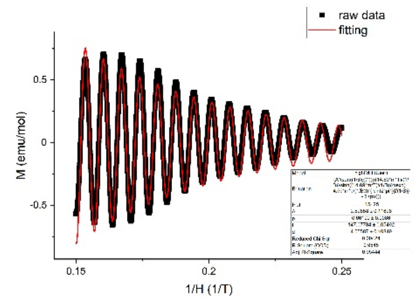

Figure 4-raw data (black) plotted against model from eq. 4 (red)

Angular Measurement

A methodology for modeling a material's fermi surface was then learned using the material $TaAl_3$. The figure on the right provides a visual to this testing. The sample is placed in the magnetometer and then a constant field is applied to the sample at different angles, essentially providing a cross-section of the fermi surface. This test produces data in the form of frequency vs. angle. The frequencies found at each angle correspond to the frequency of a band.

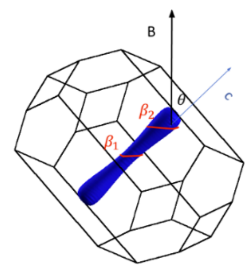

Figure 5-experimental setup for angular dependence test

The orbit frequency may change as a result of changing angle, providing insight to the shape of the fermi surface. If there is little angular change, the surface may be inferred to be spherical, whereas for cylinders, there will be more observable change in the frequency of the orbit. Thus, from the data displayed in Fig. 6, it can be expected that due to the large changes and frequencies for the β pocket, these are most likely a cylinder, but a smaller frequency and angular dependence provides evidence for a small, spherical α.

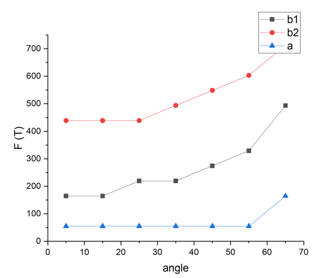

Figure 6-Frequency dependence of angle for TaAl3 bands

Then, moving onto DFT, the experimental results are compared to the fermi surface predicted by open-source .cif files. By breaking the Hamiltonian into parts and by using the gradient of the material density, DFT is able to model Fermi surfaces.

$$\hat{H}\psi = [\hat{U} + \hat{T} + \hat{V}]\psi = [\sum_i^N \left(\frac{-\hbar^2}{2m_i}\nabla_i^2\right) + \sum_i^N V(\boldsymbol{r}_i) + \sum_{i<j}^N U(\boldsymbol{r}_i, \boldsymbol{r}_j)]\psi = E\psi$$

Kinetic Energy

Potential Energy

e-e Interaction

Conducting DFT for $TaAl_3$, the following were found: band diagram, Fermi surface model, and frequency-angle relation. These can be seen in Fig. 7.

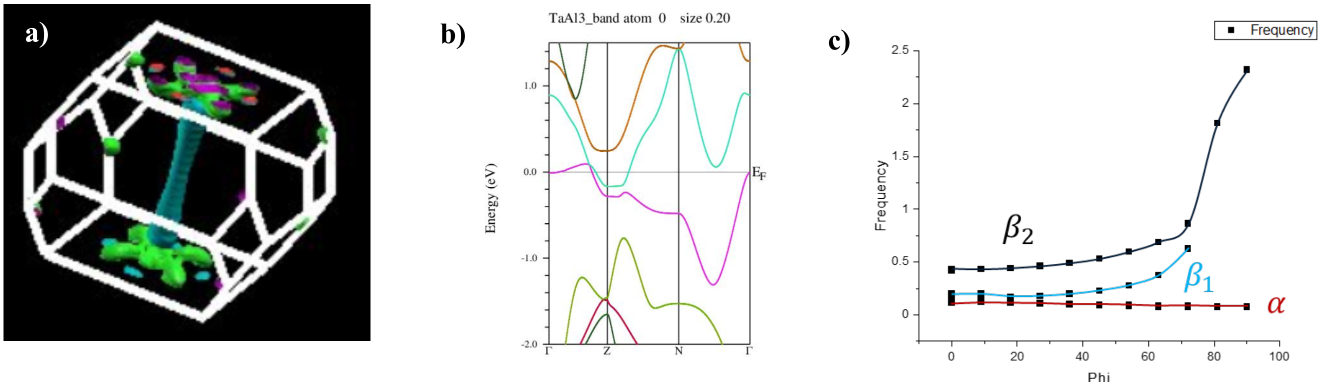

Figure 7-a) TaAl3 Fermi surface b) band diagram c)frequency-angle relationship

Just from observation, it is clear that the experimental predictions were correct. Delving further, though, Fig. 8 displays a comparison of the experimental and DFT frequency-angle data. Both show α to be fairly constant at a very low frequency while the β phases are higher frequency and steeply change with angle. Thus, this structure is confirmed.

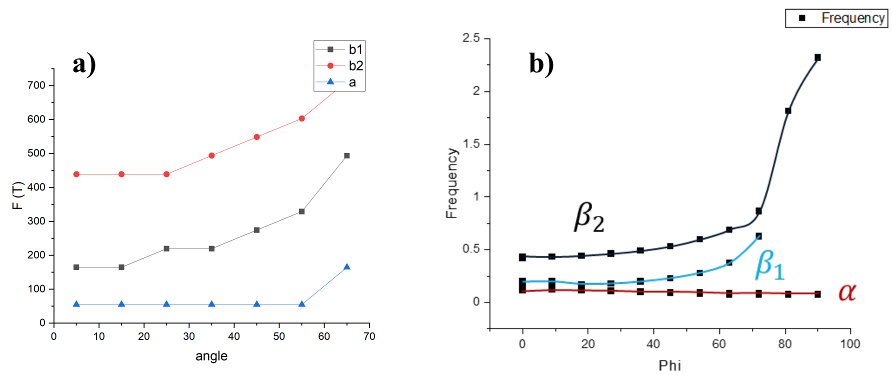

Figure 8- a) experimental data b) DFT calculated data

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[2] Chen, K.-W., et al. "Bulk Fermi Surfaces of the Dirac Type-II Semimetallic Candidates MAl3 (Where M=V, Nb, and Ta)." *Physical Review Letters*, vol. 120, no. 20, 2018, doi:10.1103/physrevlett.120.206401.

[3] Chen, K-W, et al. "Uncovering the Behavior of Hf2Te2P and the Candidate Dirac Metal Zr2Te2P." *Journal of Physics: Condensed Matter*, vol. 28, no. 14, 2016, doi:10.1088/0953-8984/28/14/14lt01.

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