Signature of nodal-line crossing in Dirac semimetal ZrSiS

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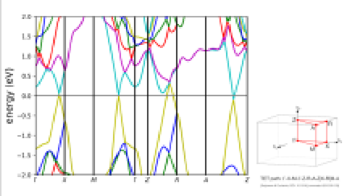
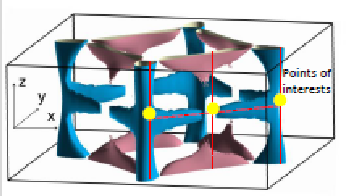
- DFT-band structure of ZrSiS without SO coupling
- Nodal line (maybe gaped) forms a cage of nodal liens in the Brillouin zone

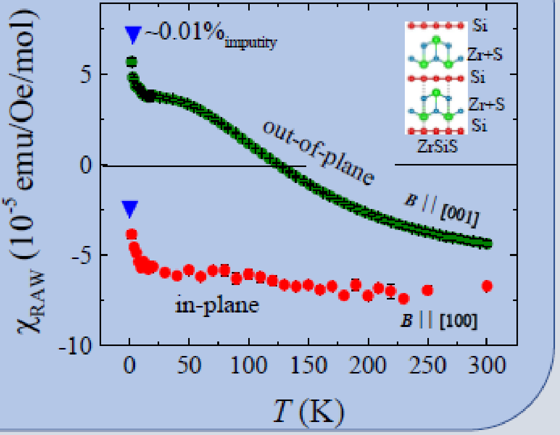


- DFT calculated Fermi surface
- Blue: hole pocket
- Red: electron pocket



- By quantum oscillations and ARES DFT calculated predicted pocked have been identified.
- Quantum oscillations reveal additional small pocket of 8.5 T, which position in the BZ is not known
- Using the angular magnetoresistance the most probable shape of DFT calculated Fermi surface has been pined down [1].

- SQUID measurements of static magnetic susceptibility revealed strong anisotropy between the in-plane and out-of-plane susceptibility
- When magnetic field in orientate in the a-b plane the susceptibility is diamagnetic and weakly temperature dependent
- The out-of-plane susceptibility shows unexpectedly strong temperature dependence and transition form diamagnetic to paramagnetic behavior
- At low field small contribution form localized magnetic moment gives an increase in the susceptibility. Estimation of 0.01% of S=1/2 impurities



Theoretical model

- In general case response form Dirac systems should be diamagnetic and almost temperature independent
- When Fermi energy is close to the Dirac point (or nodal line) magnetic susceptibility can strong increase in magnitude – „singular contribution"
- We used model developed by G.P. Mikitik and Yu.V. Sharlai* for susceptibility of nodal-line semimetals crossing points [2,

$$\varepsilon_{c,v}(\mathbf{p}) = \varepsilon_d + ap_1 + B_2p_2^2 + B_3p_3^2 + E_{c,v}(\mathbf{p}), \qquad (1)$$

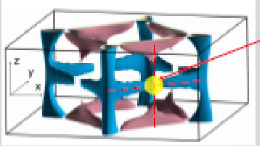
$$E_{c,v}(\mathbf{p}) = \pm\left[(a'p_1 + B_2'p_2^2 + B_3'p_3^2)^2 + \beta^2p_2^2p_3^2\right]^{1/2}, \qquad (2)$$

- **Susceptibility of the nodal-lone crossings points:**

$$\chi = \frac{\Delta\chi}{1+\exp(-\zeta/T)},$$

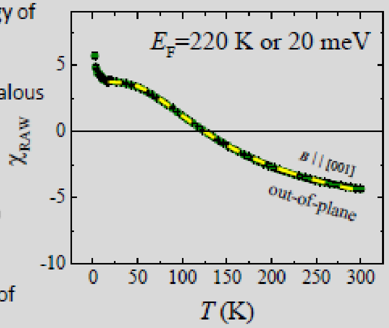
- Positive contribution for electrons and negative for holes
- If Fermi energy if far from the Dirac point the contribution is temperature independent (positive or negative)

- Electron and hole pocket obtained from DFT calculations and seen by ARPES have temperature independent contribution since Fermi energy if far from the-nodal line
- Fitting the χ(T) to the experimental data we get the Fermi energy of of 20 meV which correspond to the 8.5 T pocket
- More experiments is on the way to elucidate the origin of anomalous susceptibility response



Preliminary results:

- Anomalous contribution to χ(T) comes from 8.5 T small electron pocket
- Pocket is located at cryosection of nodal lines in $\Gamma - M - X$ plane



[1] M. Novak et al., Phys. Rev. B 100, 085137 (2019)
[2] G. P. Mikitik, Low Temp. Phys. 33, 839, (2007)
[3] G. P. Mikitik and Yu.V. Sharlai, PRB 94, 195123 (2016) and 97, 085122 (2018)

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