Experimentally hunting topology

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SCHWEIZERISCHER NATIONALFONDS
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SWISS NATIONAL SCIENCE FOUNDATION

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THE UNIVERSITY OF CALIFORNIA BERKELEY 1868 LET THERE BE LIGHT

erc

Los Alamos NATIONAL LABORATORY EST. 1943

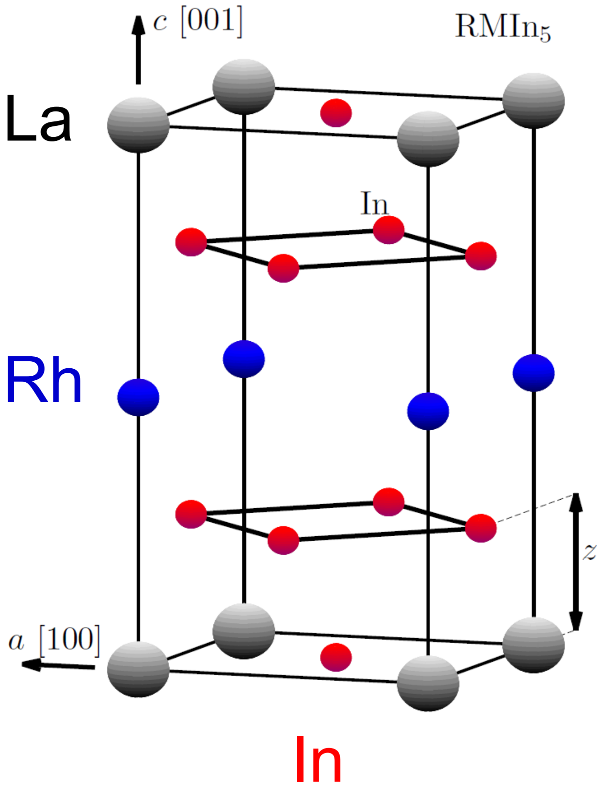
NATIONAL MAGLAB

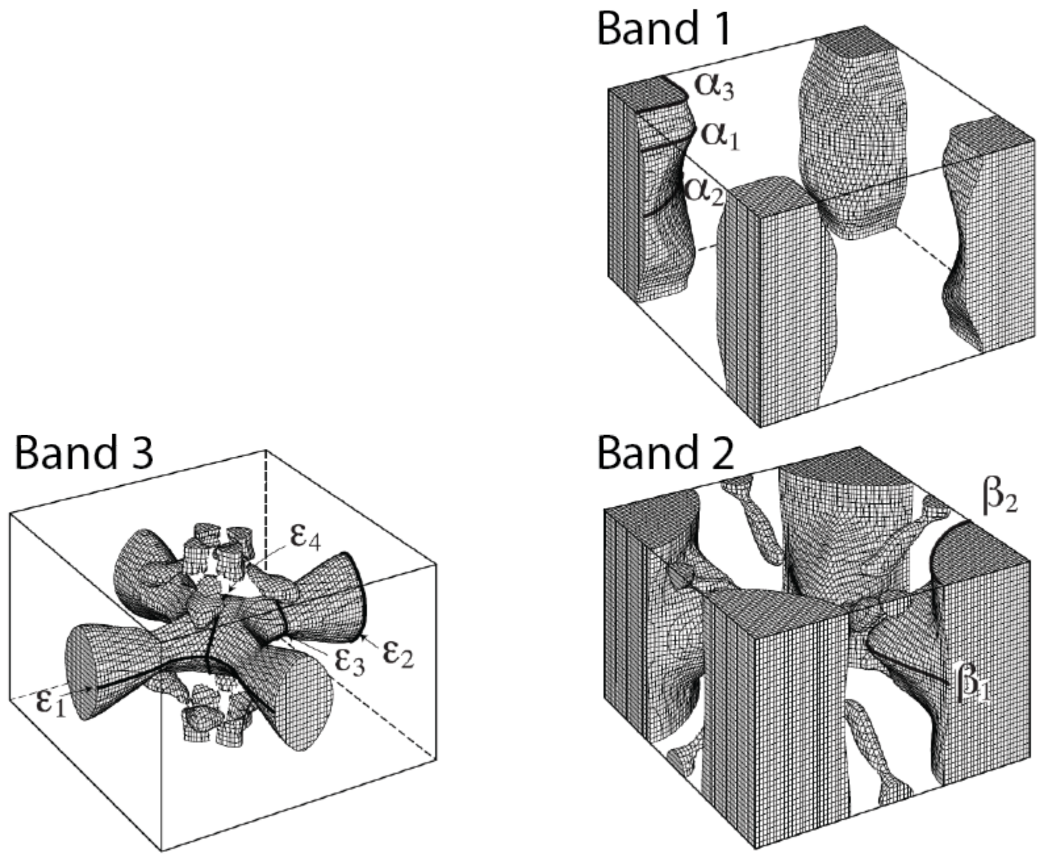
The “topology-o-meter”

Outline

- Magnetic anomaly in the quantum limit of topological semi-metals
- Phase sensitive detection
- Temperature-dependent quantum oscillations

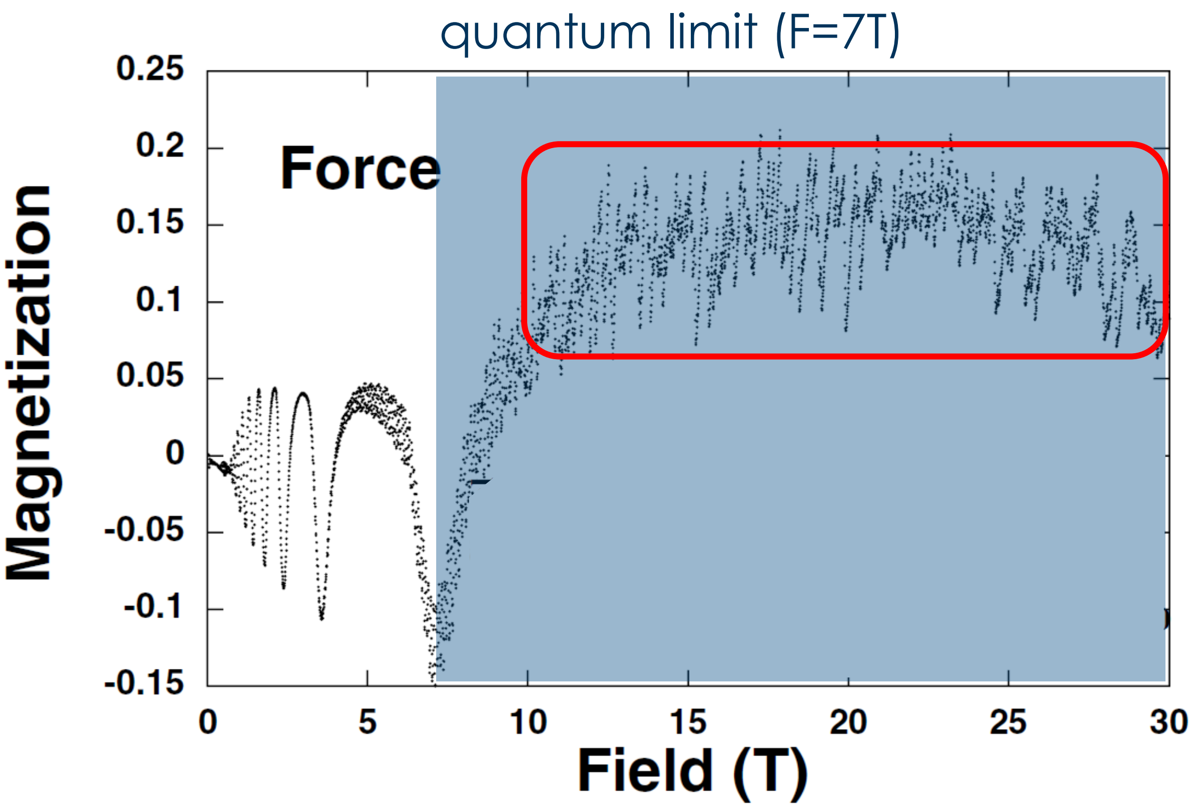
$LaRhIn_5$: complex metal & Dirac candidate

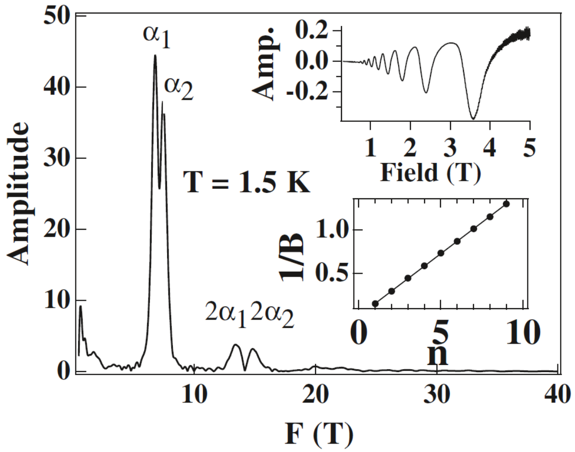




H. Shishido et al., JPSJ 71, 162 (2002)

A small frequency dominates quantum oscillations





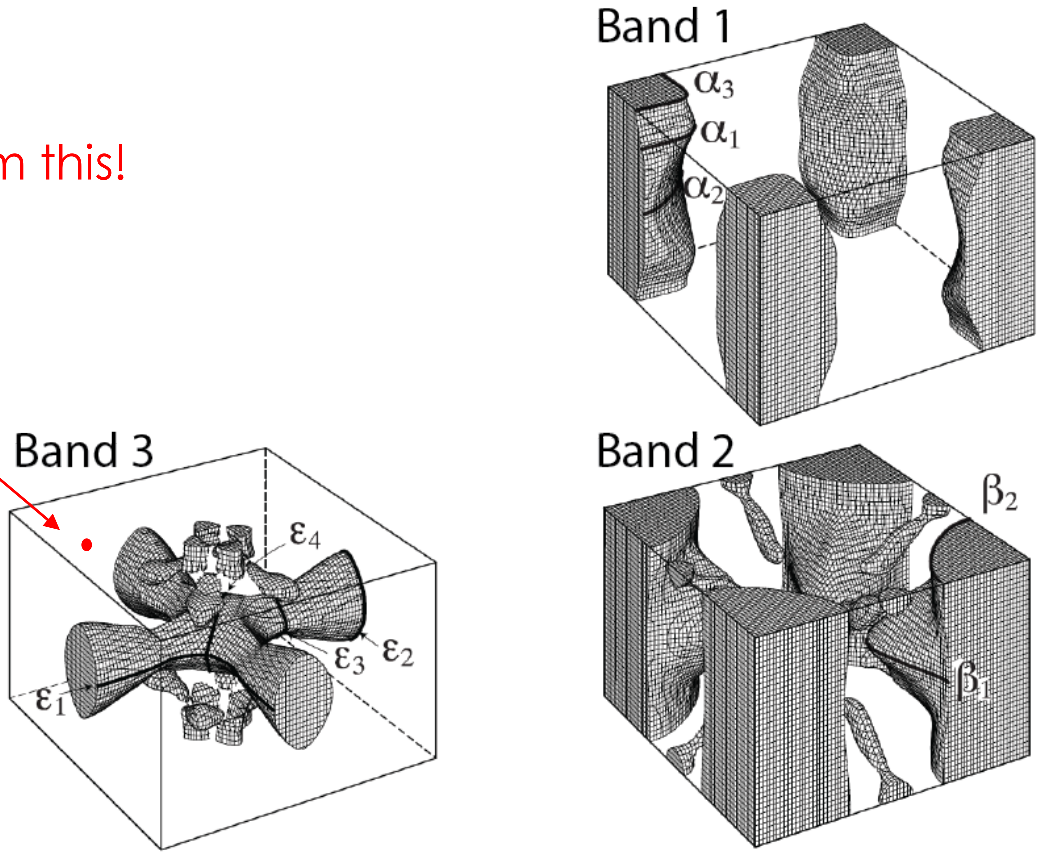
F=7T
10^{-4} of BZ

Magnetic response of $LaRhIn_5$ is completely dominated by 7T pocket, 0.1% of carriers!

R.G. Goodrich et al., PRL 89, 026401 (2002)

A small frequency dominates quantum oscillations

Magnetization only comes from this!



Magnetic response of $LaRhIn_5$ is completely dominated by 7T pocket, 0.1% of carriers!

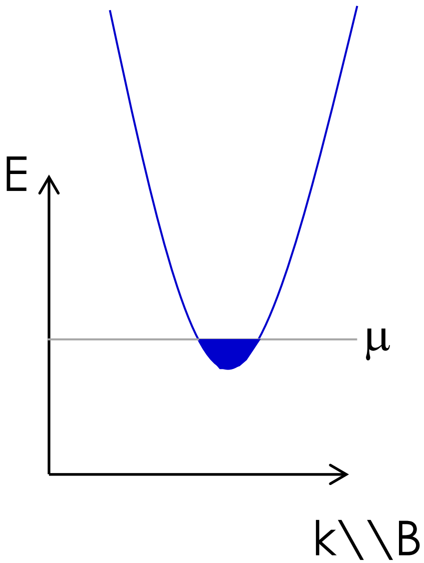
R.G. Goodrich et al., PRL 89, 026401 (2002)

This sounds odd

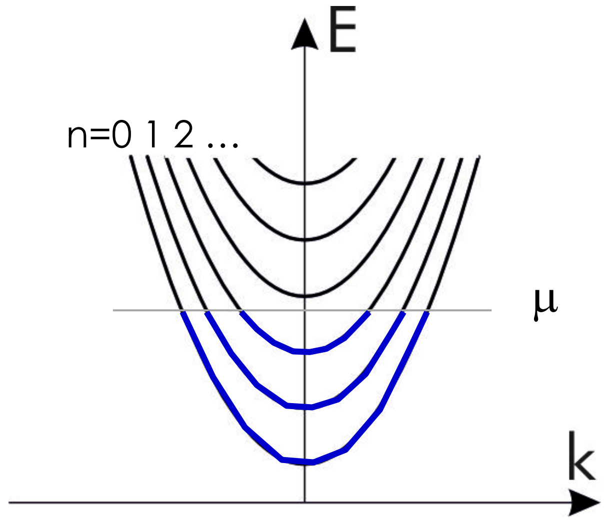
Topologically trivial electrons (Schrödinger)

Ultraquantum limit ($B>B_0$)

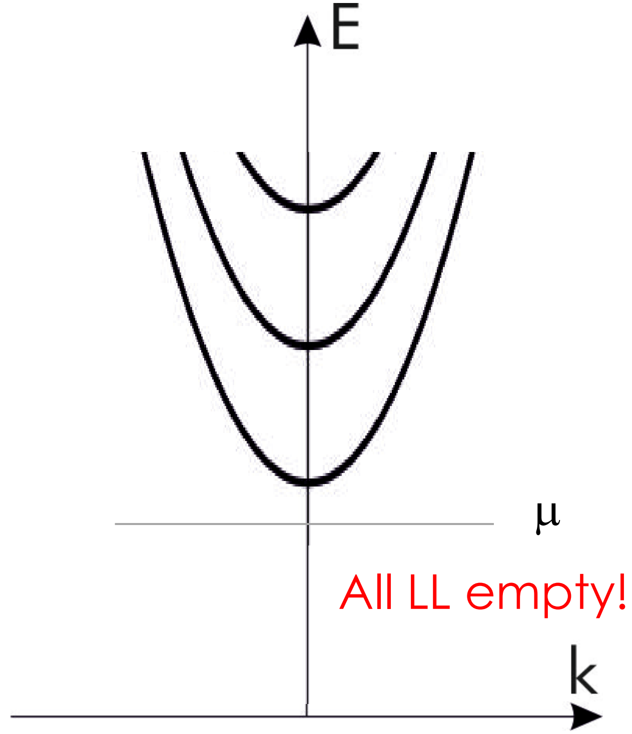
B=0



Landau levels (B>0)



$$\varepsilon_{n,k} = \hbar \frac{eB}{m}\left(n + \frac{1}{2}\right) + \frac{\hbar^2}{2m} k_z^2$$



μ constant
(it's a metal!)

How can completely empty states dominate the magnetization from 10-30T?

They cant!

G.P. Mikitik and Yu. V. Sharlai, PRL 93, 026401 (2004)

Well ahead of time!

nature

VOLUME 93, NUMBER 10 — week ending 3 SEPTEMBER 2004

Berry Phase and de Haas–van Alphen Effect in $LaRhIn_5$

G. P. Mikitik and Yu. V. Sharlai

B. Verkin Institute for Low Temperature Physics & Engineering, Ukrainian Academy of Sciences, Kharkov 61103, Ukraine

(Received 19 April 2004; published 2 September 2004)

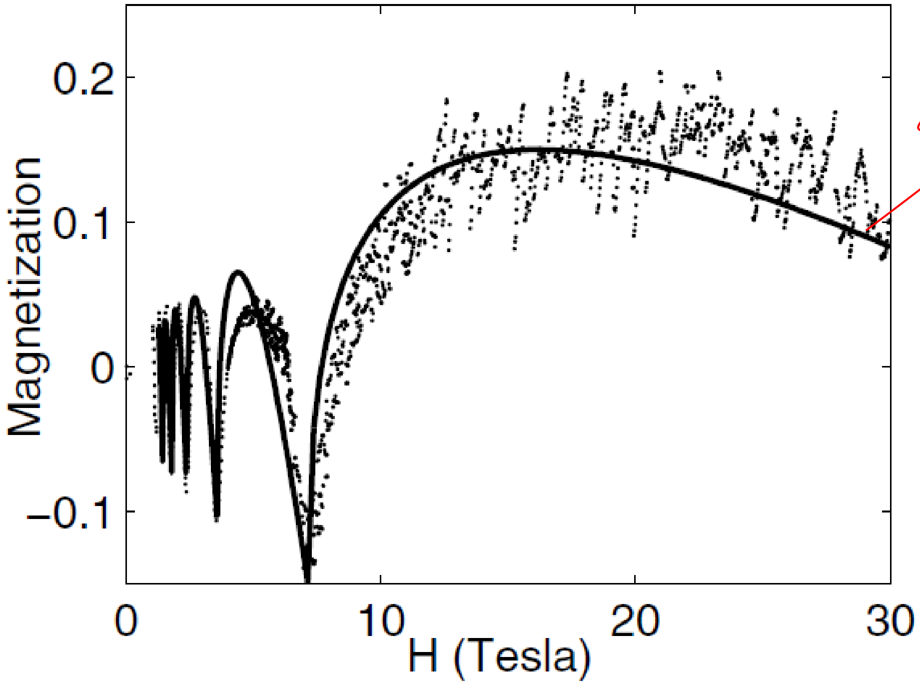
We explain the experimental data on the magnetization of $LaRhIn_5$ recently published by Goodrich *et al.* [Phys. Rev. Lett. **89**, 026401 (2002)]. We show that the magnetization of a small electron group associated with a Dirac nodal line was detected in that Letter. These data provide the first observation of the Berry phase of electrons in metals via the de Haas–van Alphen effect.

DOI: 10.1103/PhysRevLett.93.106403 PACS numbers: 71.18.+y, 03.65.Vf

G.P. Mikitik and Yu. V. Sharlai, PRL 93, 026401 (2004)

Strong evidence for Dirac Fermions

Quantitative
Dirac prediction



The magnetization of $LaRhIn_5$ is dominated by a small pocket of Dirac fermions.

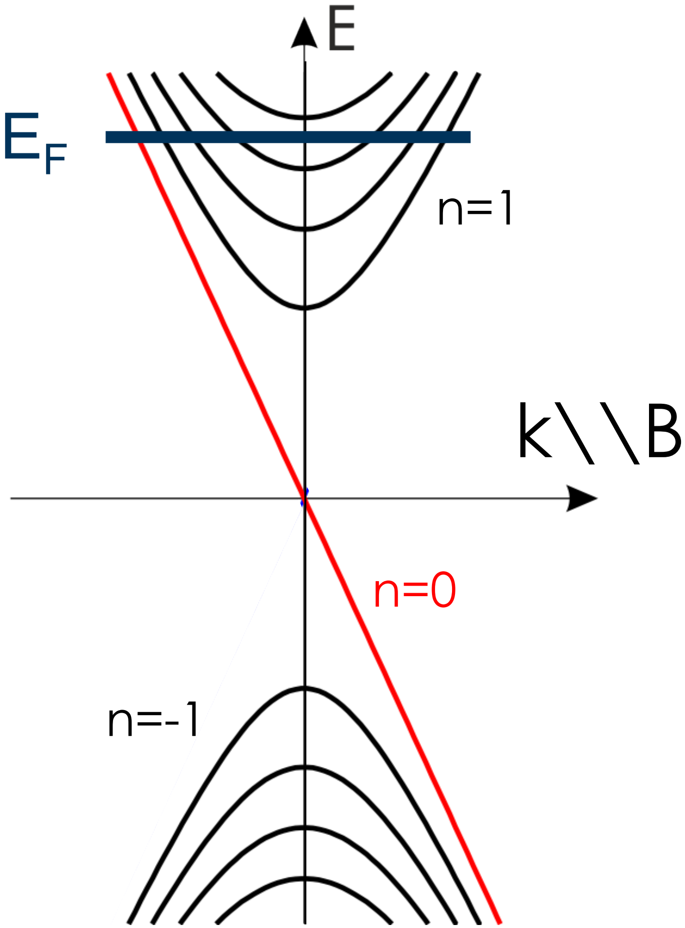
G.P. Mikitik and Yu. V. Sharlai, PRL 93, 026401 (2004)
A. Alexandradinata et al., PRX 8, 011027 (2018)

For the aficionado/a: Healthy and friendly dispute on matters arising:
Nat. Comm. 14:2061 (2023) vs Nat. Comm. 14:2060 (2023)

Landau quantization of Dirac / Weyl systems

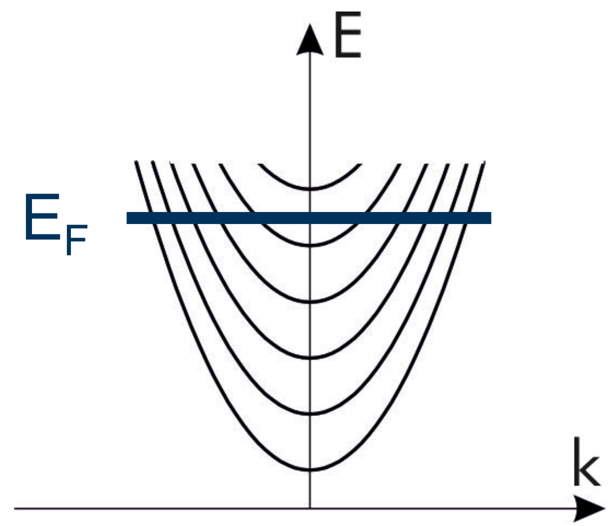
Relativistic electrons

$$\varepsilon_{n,k} = \hbar v_F \sqrt{2Bn + k_z^2}$$



Trivial electrons

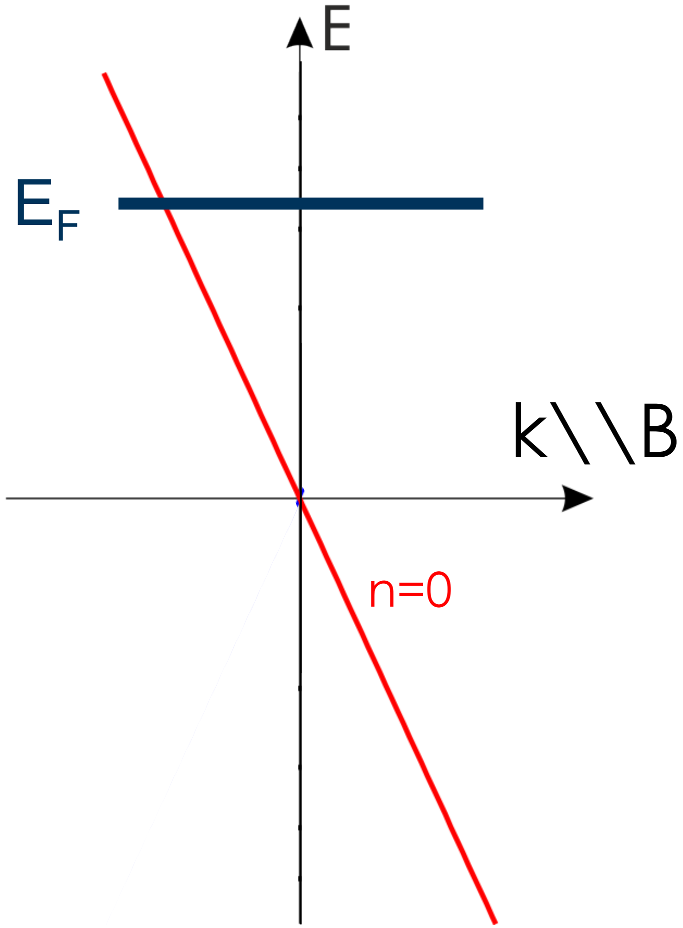
$$\varepsilon_{n,k} = \hbar \frac{eB}{m}\left(n + \frac{1}{2}\right) + \frac{\hbar^2}{2m} k_z^2$$



Topological signatures in the quantum limit

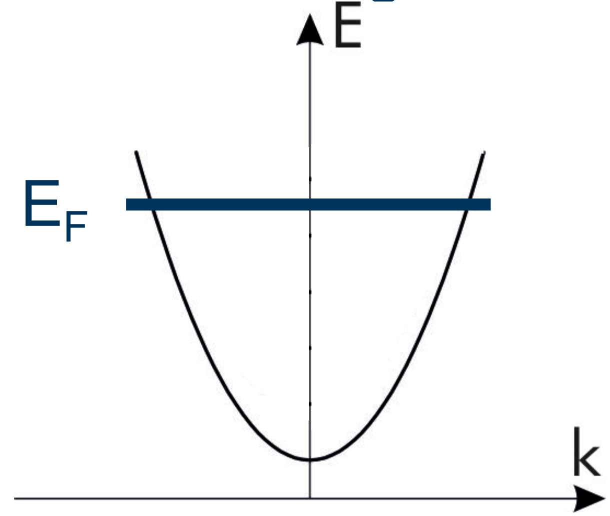
Relativistic electrons

$$\varepsilon_{n,k} = \hbar v_F \sqrt{2Bn + k_z^2}$$



Trivial electrons

$$\varepsilon_{n,k} = \hbar \frac{eB}{m}\left(n + \frac{1}{2}\right) + \frac{\hbar^2}{2m} k_z^2$$



Magnetization in the QL signals Weyl/Dirac

Relativistic electrons

$$\varepsilon_{n,k} = \hbar v_F \sqrt{2Bn + k_z^2}$$

$$M \sim \frac{\partial \varepsilon_{0,k}}{\partial \mathrm{B}} = 0$$

Trivial electrons

$$\varepsilon_{n,k} = \hbar \frac{eB}{m}\left(n + \frac{1}{2}\right) + \frac{\hbar^2}{2m} k_z^2$$

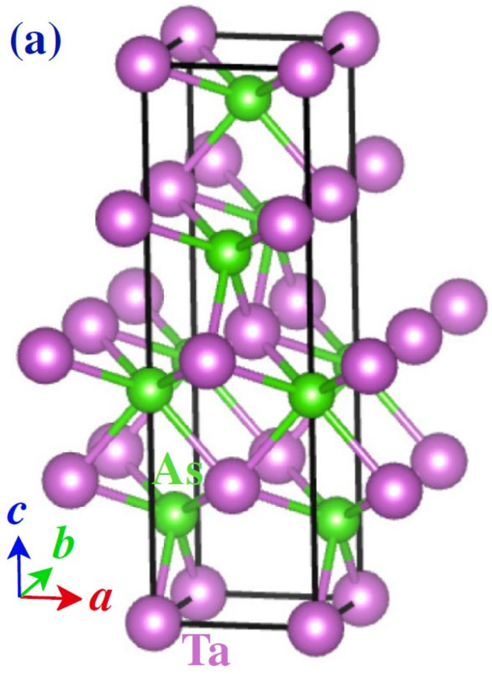
$$M \sim \frac{\partial \varepsilon_{0,k}}{\partial \mathrm{B}} \neq 0$$

$$M = -\frac{\partial F}{\partial H} \rightarrow \text{diamagnetic}$$

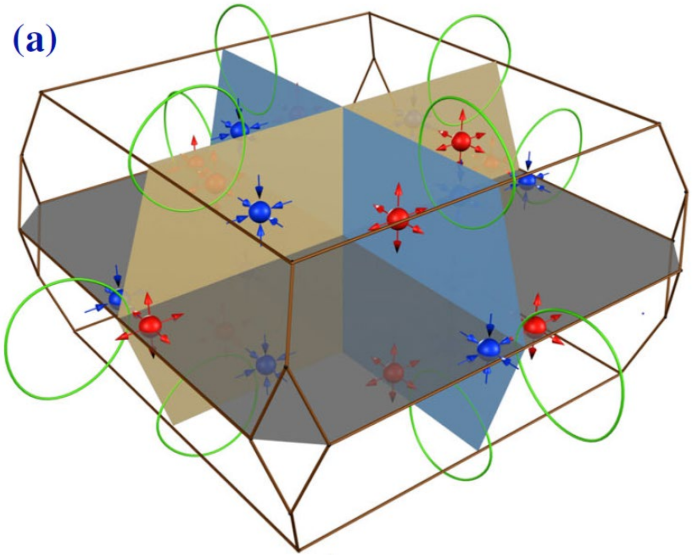
Magnetization shows distinct signature of Weyl/Dirac fermions in the quantum limit

Finding the Weyl fermions in NbAs

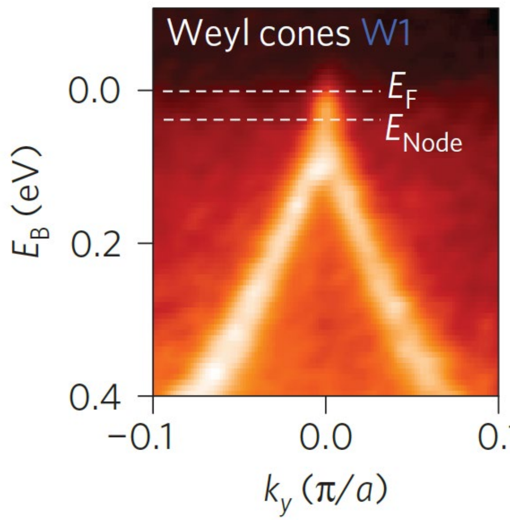
NbAs



- Non-centrosymmetric Weyl semi-metal
- Both trivial & topological FS sheets
- 24 Weyl nodes (crystal symmetry copies)

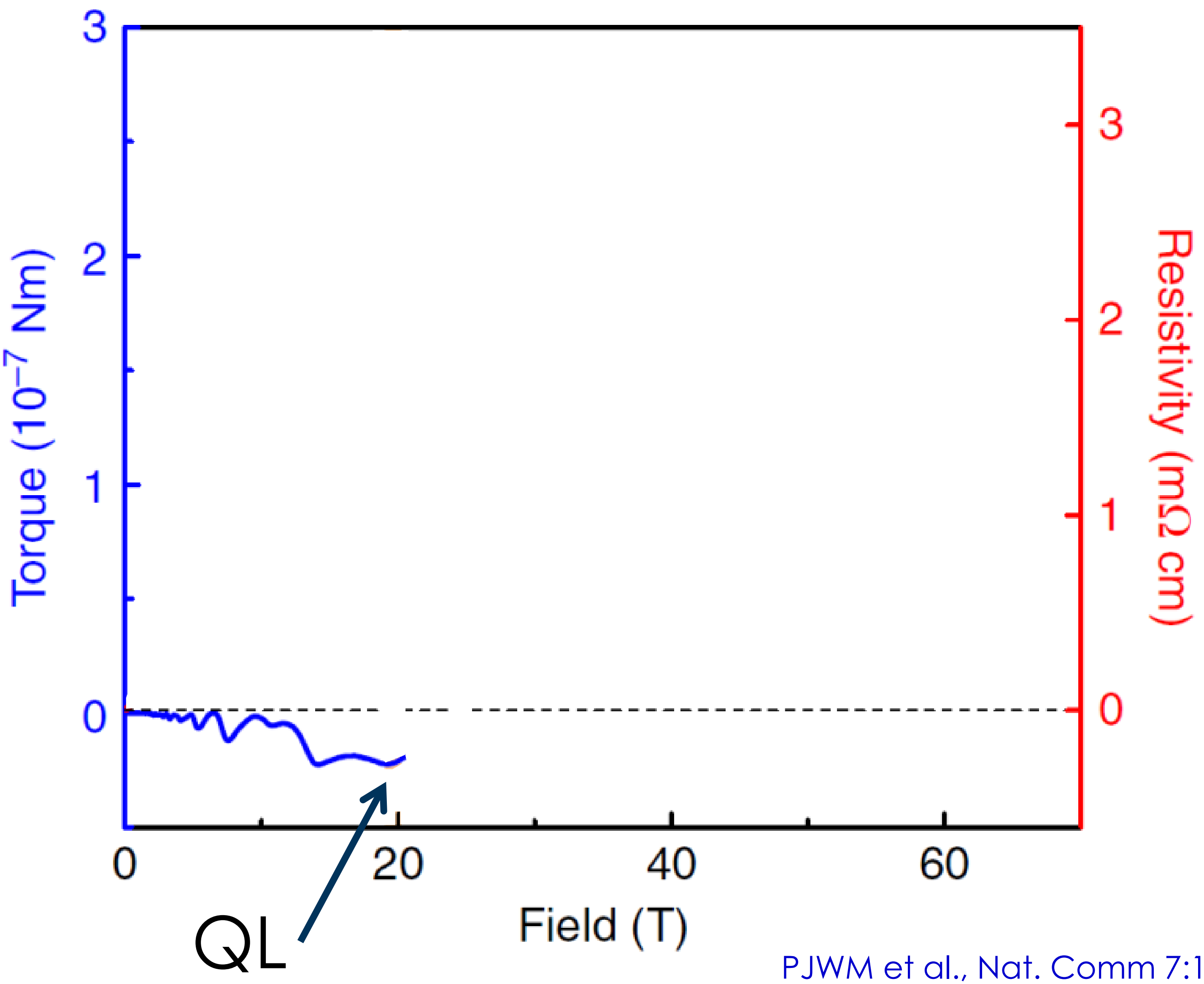


Hongming Weng et al., PRX 5, 01129 (2015)



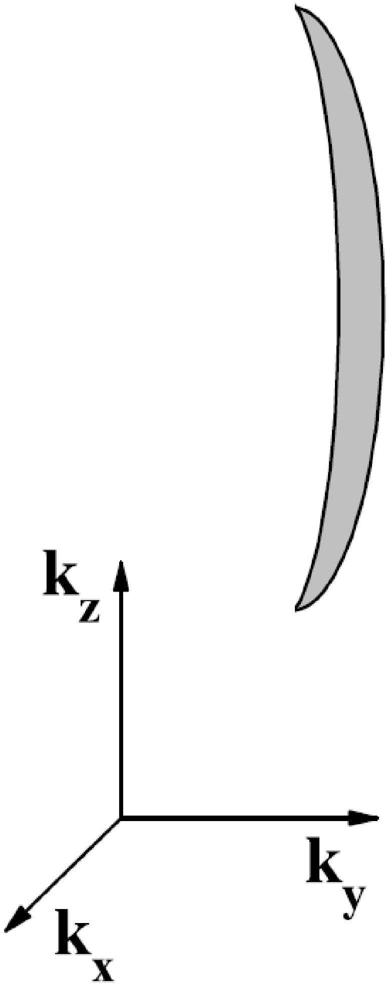
Su-Yang Xu et al., Nat.Phys.11, 748 (2015)

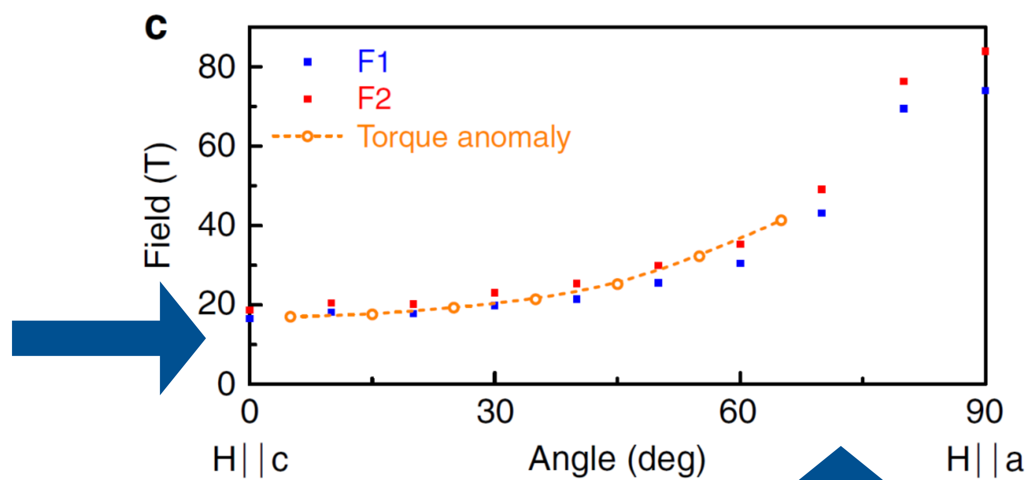
Topological torque anomaly at the quantum limit



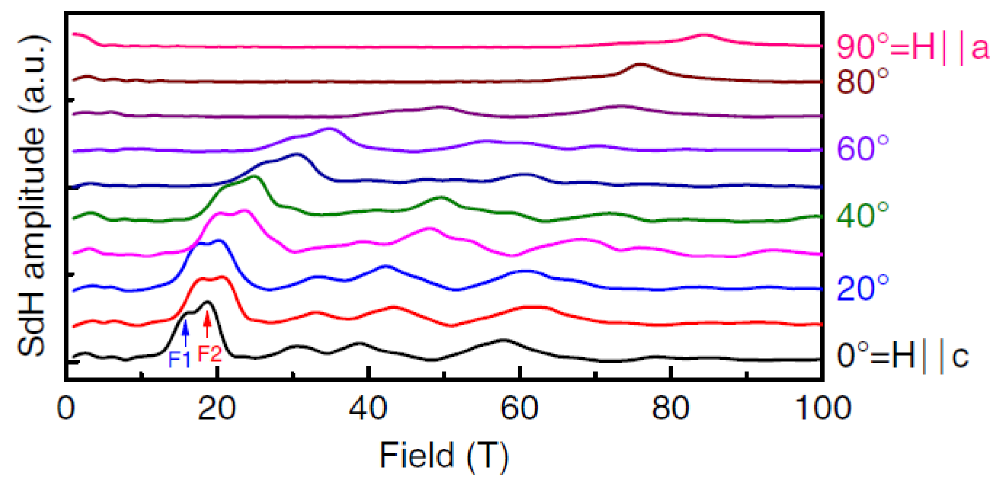
PJWM et al., Nat. Comm 7:12492 (2017)

Torque anomaly tracks the quantum limit angle

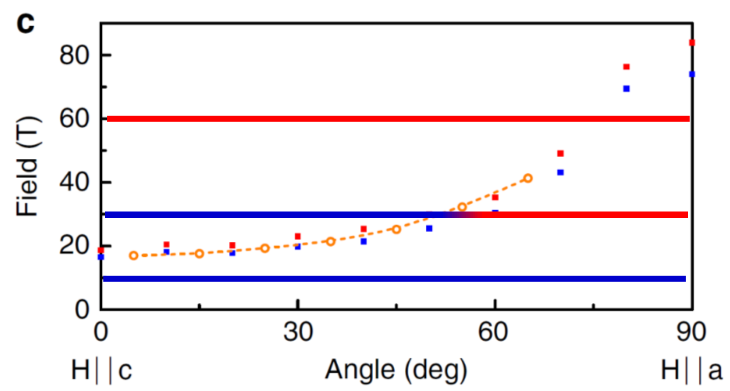


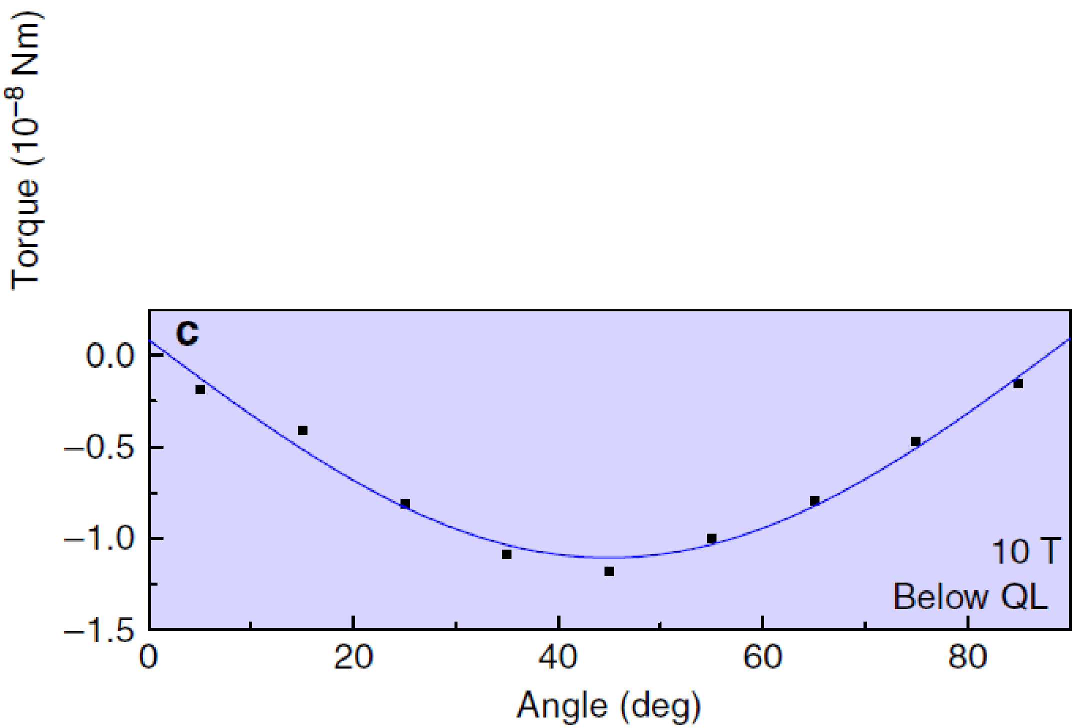


Track quantum limit
through quantum oscillations



Topological torque anomaly at the quantum limit





Berry paramagnetism

Sign change of torque
→ Sign change of M

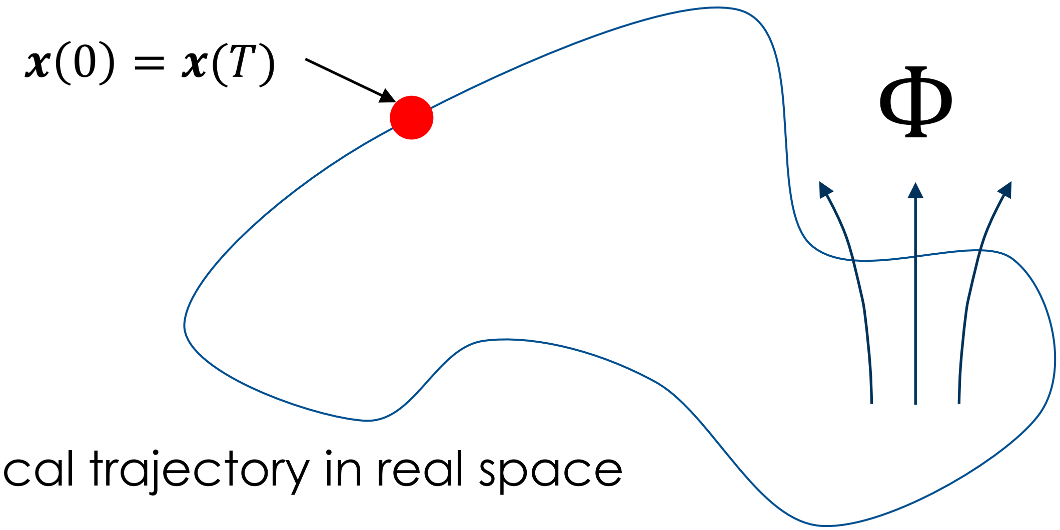
$$\tau = M \times H$$

Anomalous magnetization when Weyl / Dirac pockets reach the quantum limit. This dominates the magnetism, even when large, high density bands coexist that never reach their quantum limit.

Outline

- Magnetic anomaly in the quantum limit of topological semi-metals ✓
- Phase sensitive detection
- Temperature-dependent quantum oscillations

Quantum Electrons in a magnetic field



Closed classical trajectory in real space

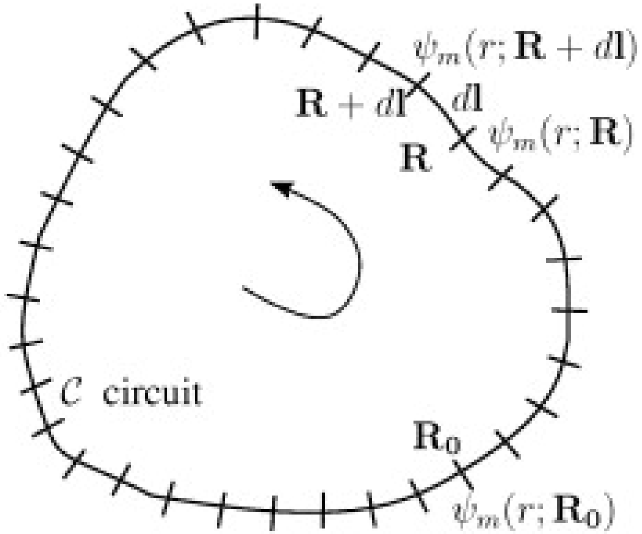
Bohr-Sommerfeld quantization: $\hbar^{-1} \oint \boldsymbol{p}\, d\boldsymbol{r} = 2\pi(n+\gamma)$

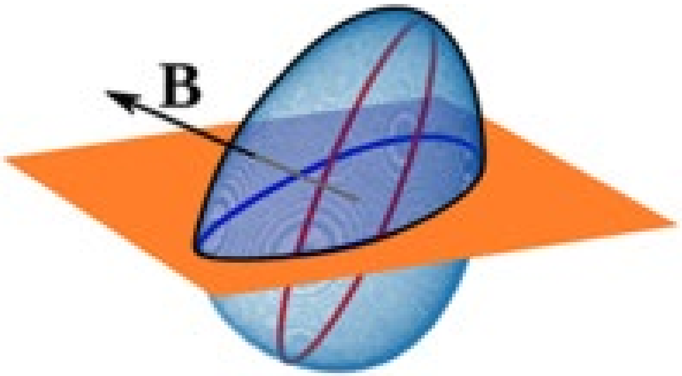
$$\boldsymbol{B} = \nabla \times \boldsymbol{A} \quad \boldsymbol{p} \rightarrow \boldsymbol{p} - e\boldsymbol{A}$$

Every flux quantum Φ_0 adds 2π to the phase.

But how about the phase offset γ?

Interferometric detection of Berry phase





Electron on a Fermi surface orbiting a topological defect is a direct probe of the Berry phase.

1. Other corrections to phase beside Berry ($\sim\hbar$)
2. Ill-defined problem due to degeneracies

Dirac semi-metal Cd_3As_2 : «anomalous» quantum oscillation phase

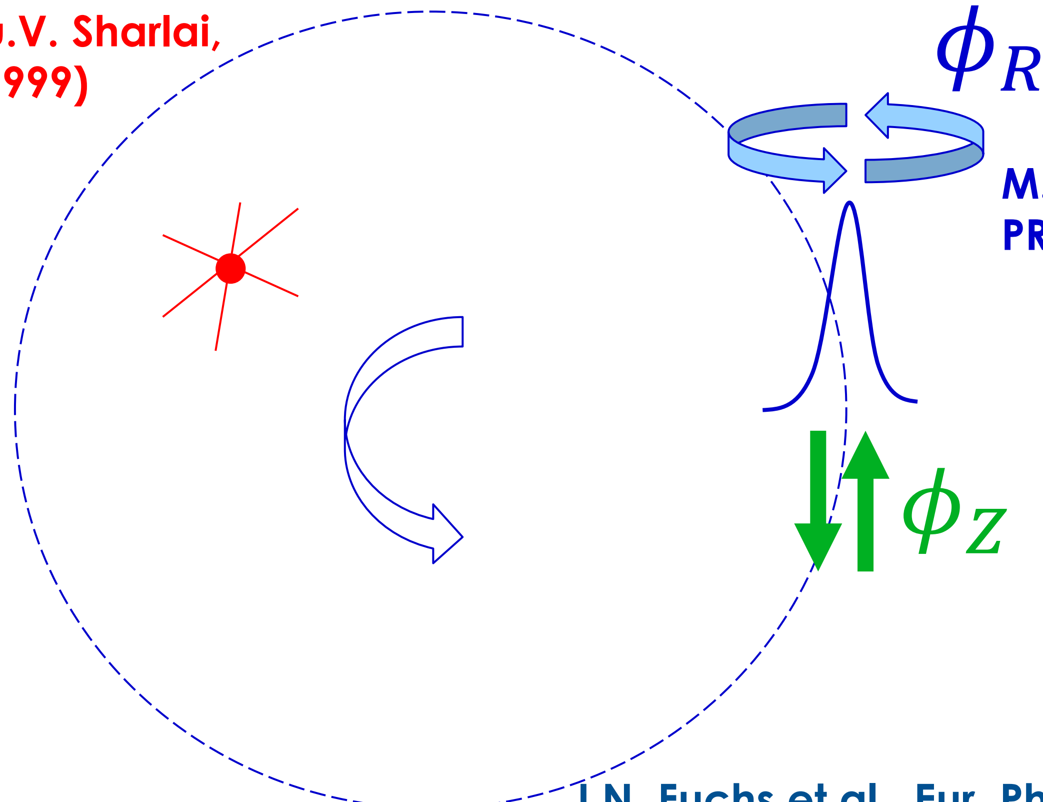
L.P. He et al., PRL 113, 246402 (2014)

π

Maslov

J.B. Keller,
Ann. Phys. (N.Y.) 4, 180 (1958)

G.P. Mikitik, Yu.V. Sharlai,
PRL 82, 2147 (1999)



M.-C. Chang, Q. Niu,
PRB 53, 7010 (1996)

$\otimes$ B

J.N. Fuchs et al., Eur. Phys. J. B 77, 351 (2010)
A. Alexandridanata et al., PRX 8, 011027 (2018)

Spin zero

$$M_{osc} = M_{3D}\, R^{LK} \sin\left(2\pi\left(\frac{F}{B} - \gamma\right)\right)$$

$$R^{LK} = R_D\, R_T\, R_S$$

Dingle damping
Finite lifetime from scattering

Thermal damping
Fermi-Dirac broadening

Spin damping
Interference of spin up/down Fermi surfaces

$$R_D = \exp\left(-\alpha \frac{m^* T_D}{m_e B}\right)$$

$$R_T = X/\sinh(X)$$

$$R_S = \cos\left(\frac{\pi g m^*}{2 m_e}\right)$$

$$\alpha = \frac{2\pi^2 m_e k_B}{e\hbar} \sim 14.9\, T/K$$

$$X = 2\pi^2 \frac{m^*}{m_e} \frac{k_B T}{\hbar \omega_c}$$

$T_D = \frac{\hbar}{\tau k_B}$: Dingle temperature

Spin zero

$$M_{osc} = M_{3D}\, R^{LK} \sin\left(2\pi\left(\frac{F}{B} - \gamma\right)\right)$$

$$R^{LK} = R_D\, R_T\, R_S$$

Spin damping
Interference of spin up/down Fermi surfaces

$$R_S = \cos\left(\frac{\pi g m^*}{2 m_e}\right)$$

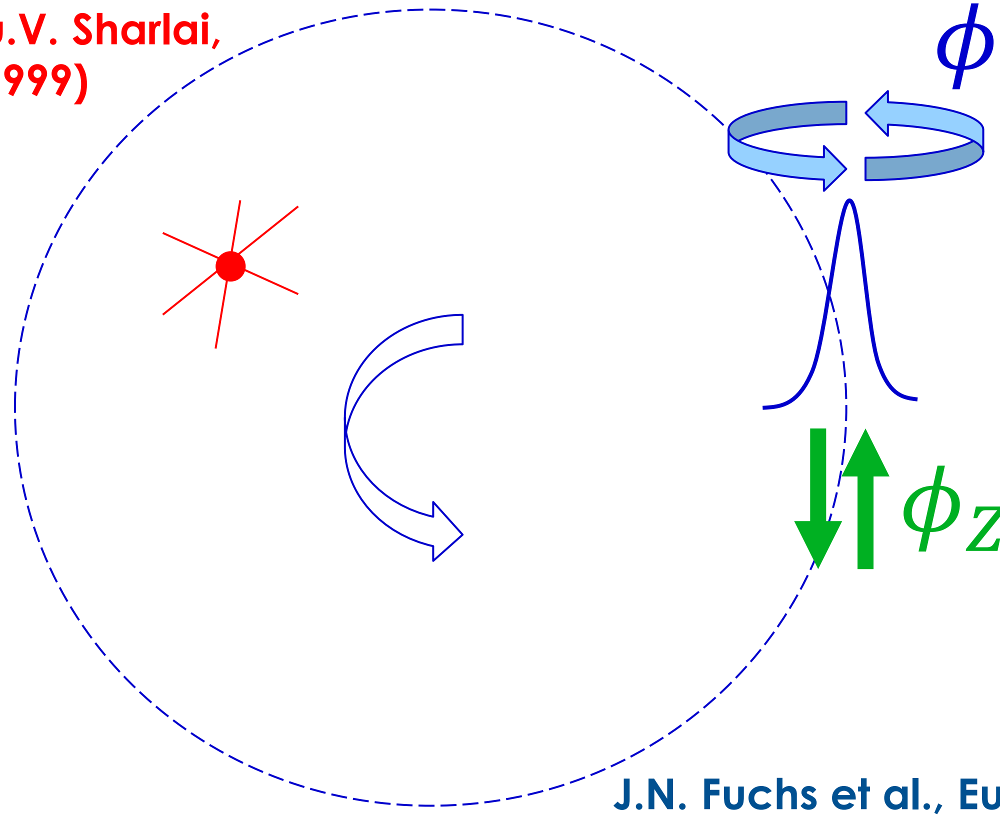
- Famous suppression of QO: **spin zero**
- dangerous: **sign change** (= π phase!)
- **Beware of circular arguments!**
  DFT g-factor → phase analysis → confirm DFT

π

Maslov
J.B. Keller,
Ann. Phys. (N.Y.) 4, 180 (1958)

G.P. Mikitik, Yu.V. Sharlai,
PRL 82, 2147 (1999)

Topology



ϕ_R Closeby bands

M.-C. Chang, Q. Niu,
PRB 53, 7010 (1996)

ϕ_Z Spin interference

$\otimes$ B

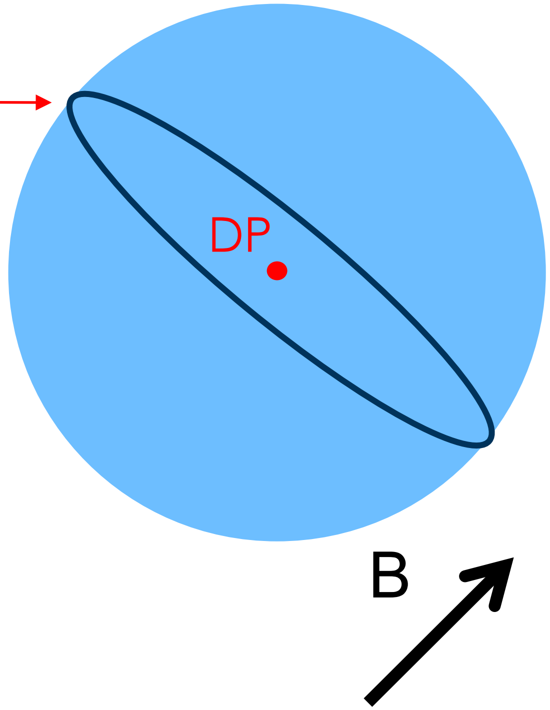
J.N. Fuchs et al., Eur. Phys. J. B 77, 351 (2010)
A. Alexandridanata et al., PRX 8, 011027 (2018)

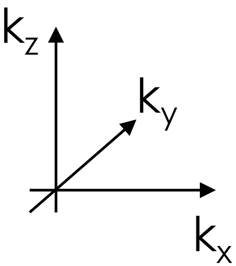
Key point 2: Degeneracies

$\psi_1(k), \psi_2(k), \ldots, \psi_D(k)$

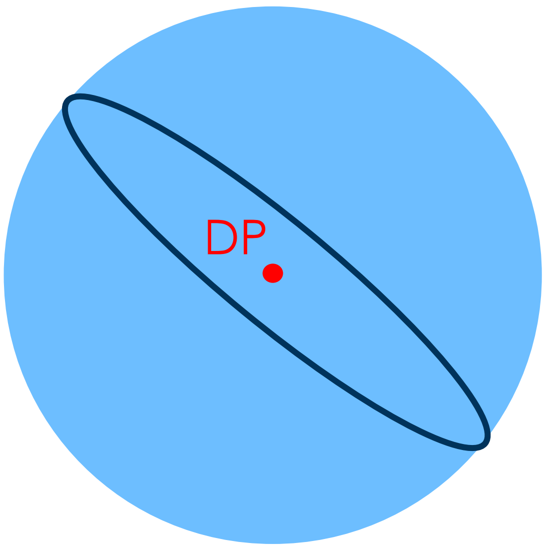
Each state on orbit D-fold degenerate in k-space (*a*=1..D)

e.g. D=2: spin-degenerate orbit





Crystal-symmetry related copies of Fermi surfaces



Symmetry of the crystal

$\neq$

Symmetry of the orbit!

λ_a^i — i^{th} orbit, a^{th} wavefunction

A. Alexandridanata et al., PRX 8, 011027 (2018)

Too many degrees of freedom!

Theory

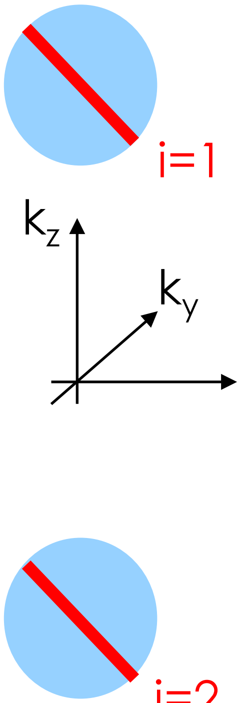
$$\Delta M \sim \sin\left(\frac{F}{B} + \lambda_1\right) + \sin\left(\frac{F}{B} + \lambda_2\right) + \sin\left(\frac{F}{B} + \lambda_3\right) + \sin\left(\frac{F}{B} + \lambda_4\right) + \ldots$$

Each orbit contributes an oscillatory component at same frequency...
... but a priori different phase!

Experiment

$$= \sin\left(\frac{F}{B} + \Theta\right)$$

Crystal symmetry reduces degrees of freedom



Preserves sign? Time reversal?

	u	s	Symmetry constraints		λ
(I) $\forall \boldsymbol{k}^{\perp}, \boldsymbol{k}^{\perp} = g \circ \boldsymbol{k}^{\perp}$	0	0	$\mathcal{A} = \bar{g}\mathcal{A}\bar{g}^{-1}$	$\bar{g}^2 = e^{i\pi F\mu - i\boldsymbol{k}\cdot\boldsymbol{R}}$	$\cdots$
	0	1	$\mathcal{A} = \bar{g}\mathcal{A}^*\bar{g}^{-1}$	$(\bar{g}K)^2 = e^{i\pi F\mu - i\boldsymbol{k}\cdot\boldsymbol{R}}$	$e^{i\sum_a \lambda_a} \in \mathbb{R}$
(II-A) $\boldsymbol{k}^{\perp} \in \mathfrak{o}, \lvert\mathfrak{o}\rvert = \lvert g\circ\mathfrak{o}\rvert$	0	0	$\mathcal{A} = \bar{g}\mathcal{A}\bar{g}^{-1}$	$\bar{g}^N = \mathcal{A}^{\pm N/L} e^{i\pi F\mu}$	$\cdots$
	0	1	$\mathcal{A} = \bar{g}\mathcal{A}^*\bar{g}^{-1}$	$(\bar{g}K)^N = \mathcal{A}^{\pm N/L} e^{i\pi F\mu}$	$e^{i\sum_a \lambda_a} \in \mathbb{R}$
	1	0	$\mathcal{A} = \bar{g}\mathcal{A}^{-1}\bar{g}^{-1}$	$\bar{g}^N = e^{i\pi F\mu - i\boldsymbol{k}\cdot\boldsymbol{R}}$	$e^{i\sum_a \lambda_a} \in \mathbb{R}$
	1	1	$\mathcal{A} = \bar{g}\mathcal{A}^t\bar{g}^{-1}$	$(\bar{g}K)^N = e^{i\pi F\mu - i\boldsymbol{k}\cdot\boldsymbol{R}}$	$\cdots$
(II-B) $\boldsymbol{k}^{\perp} \in \mathfrak{o}, \lvert\mathfrak{o}\rvert \neq \lvert g\circ\mathfrak{o}\rvert$	0	0	$\mathcal{A}_{i+1} = \bar{g}_i\mathcal{A}_i\bar{g}_i^{-1}$	$\bar{g}_N \ldots \bar{g}_1 = e^{i\pi F\mu - i\boldsymbol{k}\cdot\boldsymbol{R}}$	$\{\lambda_a^{i+1}\} = \{\lambda_a^i\}$
	0	1	$\mathcal{A}_{i+1} = \bar{g}_i\mathcal{A}_i^*\bar{g}_i^{-1}$	$\bar{g}_N K \ldots \bar{g}_1 K = e^{i\pi F\mu - i\boldsymbol{k}\cdot\boldsymbol{R}}$	$\{\lambda_a^{i+1}\} = \{-\lambda_a^i\}$
	1	0	$\mathcal{A}_{i+1} = \bar{g}_i\mathcal{A}_i^{-1}\bar{g}_i^{-1}$	$\bar{g}_N \ldots \bar{g}_1 = e^{i\pi F\mu - i\boldsymbol{k}\cdot\boldsymbol{R}}$	$\{\lambda_a^{i+1}\} = \{-\lambda_a^i\}$
	1	1	$\mathcal{A}_{i+1} = \bar{g}_i\mathcal{A}_i^t\bar{g}_i^{-1}$	$\bar{g}_N K \ldots \bar{g}_1 K = e^{i\pi F\mu - i\boldsymbol{k}\cdot\boldsymbol{R}}$	$\{\lambda_a^{i+1}\} = \{\lambda_a^i\}$

A. Alexandridanata et al., PRX 8, 011027 (2018)

3D DSM Cd_3As_2: zero-sum rule for each orbit: $\lambda_1^i + \lambda_2^i = 0$

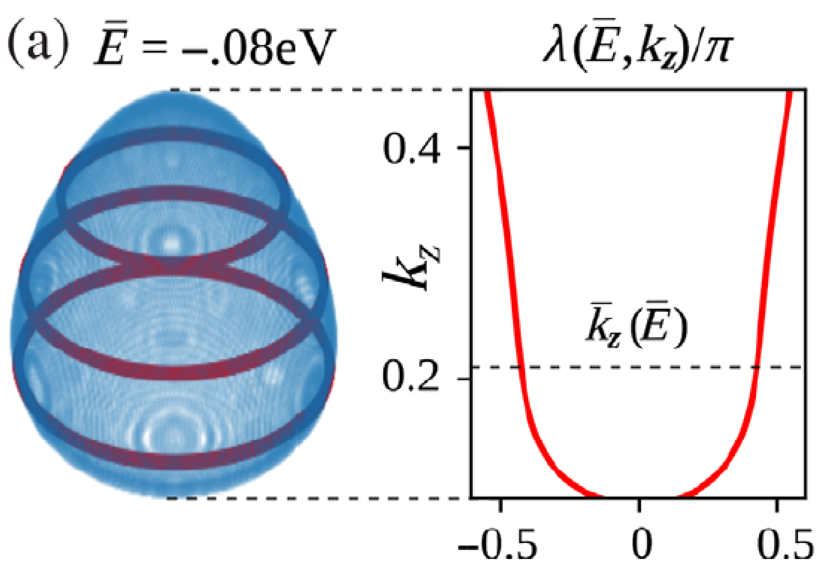
Crystal symmetry reduces degrees of freedom

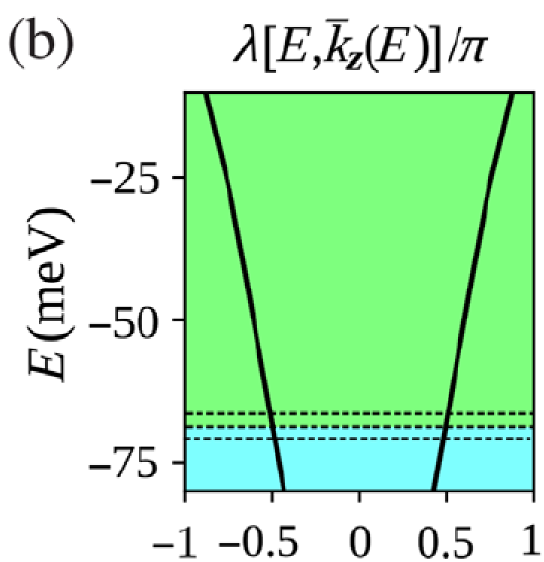
Experimental phase

$$\Theta := \frac{\lambda_1 + \lambda_2}{2} + \pi\left(1 - \mathrm{sign}\left[\cos\left(\frac{\lambda_1 - \lambda_2}{2}\right)\right]\right)/2$$

$$\Theta = \pi\left(1 - sign(\cos(\lambda_1))\right)/2$$

In the 3D DSM, both π and 0 are possible experimental phases.





$\Theta = \pi$

$\Theta = 0$

The phase is always a problem

THE DE HAAS–VAN ALPHEN EFFECT*

III. EXPERIMENTS AT FIELDS UP TO 32 kG

By J. S. DHILLON AND D. SHOENBERG, F.R.S.†
National Physical Laboratory of India, New Delhi

(*Received* 22 *October* 1954)

The periodic field dependence of magnetic anisotropy (de Haas–van Alphen effect) has been studied for bismuth and zinc crystals by the torque method between about 1·5 and 32 kG at 4·19° K and about 1·5° K; in each case the orientation was chosen so that only a single fundamental periodicity was present. Particular attention was paid to the phase and harmonic content of the oscillations and to the form of the field dependence of amplitude. For bismuth good agreement was found with the theoretical formula except that the signs of the fundamental and the odd harmonics had to be reversed. For zinc the field dependence of amplitude at high fields was quite at variance with

Bi is a **topologically trivial semi-metal**,
yet shows a quantum oscillation phase of π!

Quantum oscillation phase analyses are DANGEROUS!

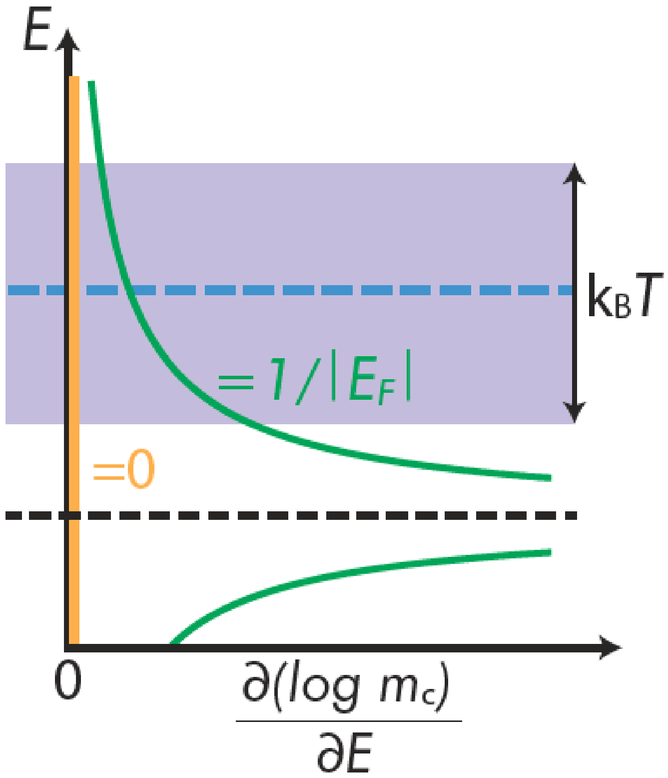
A. Alexandradinata et al., PRX 8, 011027 (2018)

Outline

- Magnetic anomaly in the quantum limit of topological semi-metals ✓
- Phase sensitive detection X
- Temperature-dependent quantum oscillations

The *effective mass* of Dirac Fermions is energy dependent

Temperature-dependent quantum oscillation frequency



Temperature damping

$$R_T = \frac{X}{\sinh(X)}; X = \frac{2\pi^2 k_B T m^*}{eB}$$

Quantum oscillations of lighter electrons are less dampened.

Effective oscillation frequency is reduced as temperature is increased.

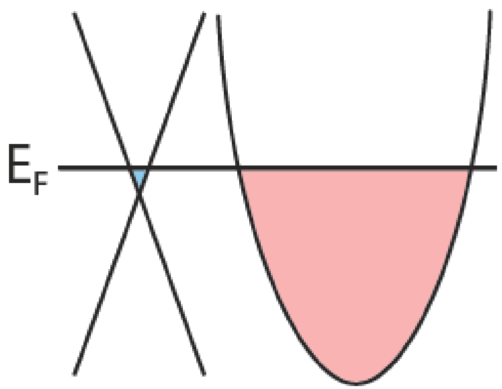
$$F_0(\mu) \rightarrow F(\mu, T) = F_0(\mu) - \frac{\pi^2}{4}\frac{(k_B T)^2}{\beta}\frac{\partial(\log m_c)}{\partial E}$$

C. Guo, A. Alexandradinata et al., Nat. Comm. 12:6213 (2021)

Dirac metals vs Dirac semi-metals

Pockets coexist with large FS

LaRhIn$_5$

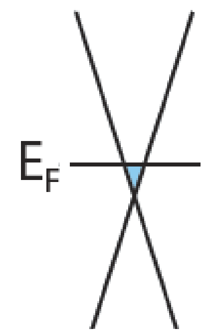


"μ constant"

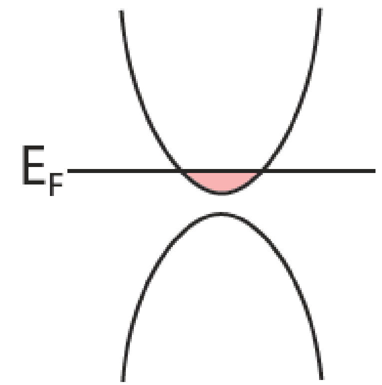
$$\Delta F = \Delta F^{top}$$

Isolated small pockets

Cd_3As_2



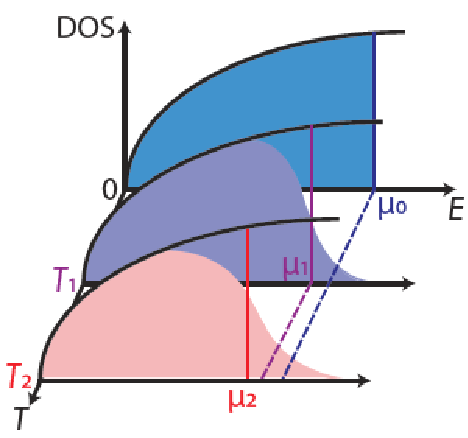
Bi_2O_2Se



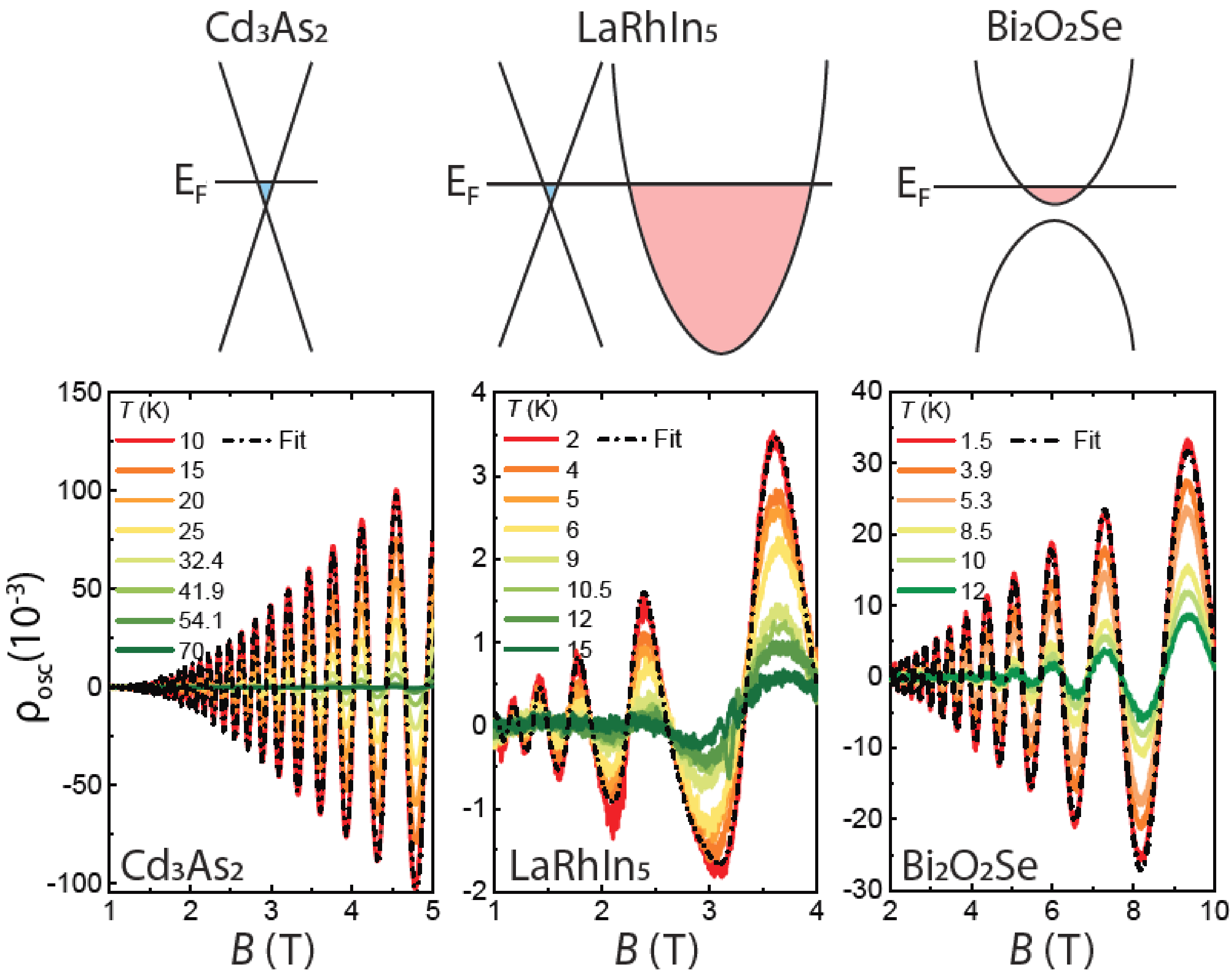
n constant

$$\Delta F = \Delta F^{top} + \Delta F^{s}$$

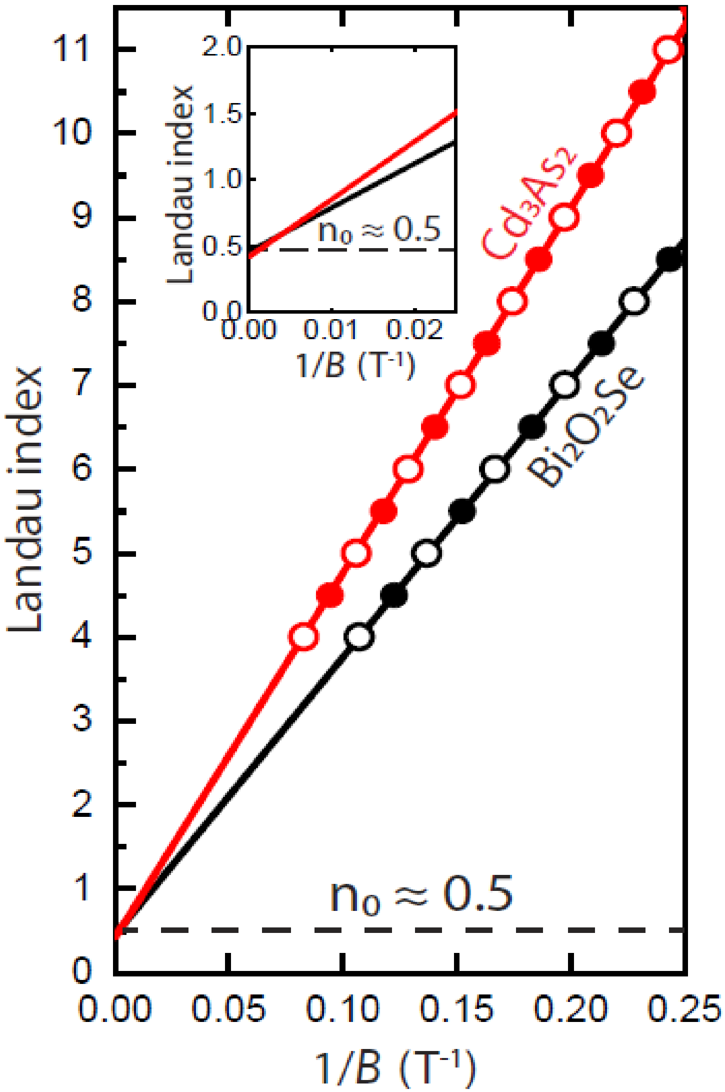
(b) Sommerfeld contribution



Benchmark the theory



Be aware of Landau fans in topological semi-metals

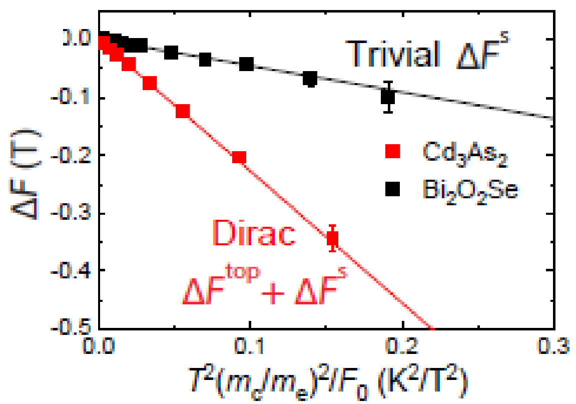


Bi_2O_2Se is a trivial semi-conductor!

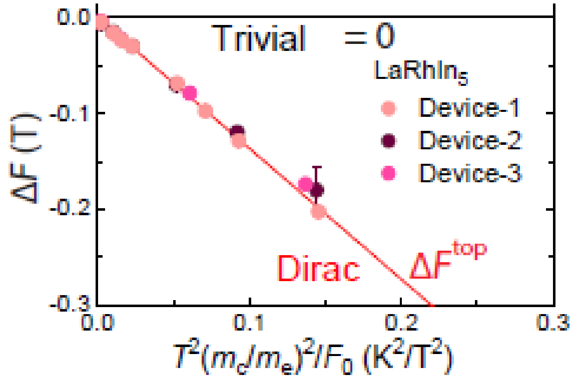
Sign change is entirely due to SOC in Bi.

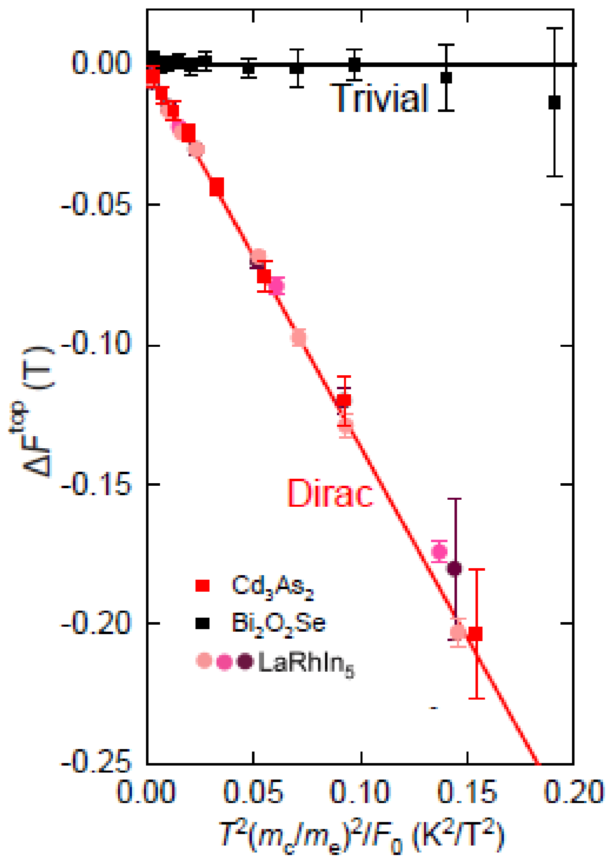
Universal behavior of topological fermions

Isolated small pockets



Pockets coexist with large FS





Great tool to fingerprint topological defects with quantum oscillations.

Outline

See all our research & find interesting PD and PhD opportunities

- Magnetic anomaly in the quantum limit of topological semi-metals ✓
- Phase sensitive detection X
- Temperature-dependent quantum oscillations ~

Some refs: **Temperature dependent quantum oscillations** – C. Guo, A. Alexandradinata et al., Nat. Comm. 12:6213 (2021), F. Yang et al., PRB 108, 035137 (2023); **Phase determination in top. Systems** - J.N. Fuchs et al., Eur. Phys. J. B 77, 351 (2010), A. Alexandridanata et al., PRX 8, 011027 (2018); **Berry phase in $LaRhIn_5$** - G.P. Mikitik and Yu. V. Sharlai, PRL 93, 026401 (2004), Nat. Comm. 14:2061 (2023), C. Guo et al., Nat. Comm. 14:2060 (2023); **Magnetic anomaly in quantum limit** - R.G. Goodrich et al., PRL 89, 026401 (2002), PJWM et al., Nat. Comm 7:12492 (2017)