



Workshop Topological Quantum Matter, KITP-UCSB Oct. 2016

The chiral anomaly in Dirac and Weyl Semimetals



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1. Chiral anomaly in Na_3Bi and the half-Heusler GdPtBi
2. Thermopower of Weyl fermions
3. Prelim results on nonsymmorphic semimetal KHgSb

Search for (3+1)d Dirac cones with protected nodes

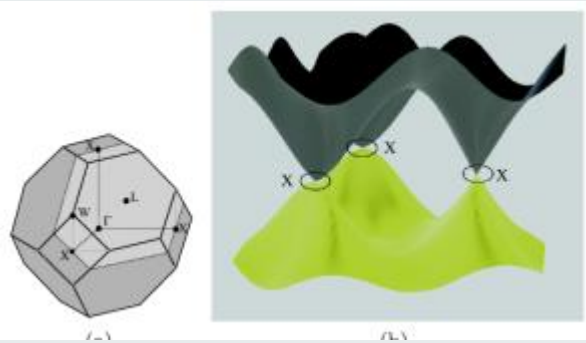
Topological semimetal and Fermi-arc surface states in pyrochlore iridates

Wan, Turner, Vishwanath and Savrasov, PRB 2011

Dirac Semimetal in Three Dimensions

Young, Zaheer, Teo, Kane, Mele and Rappe

PRL 2012



Time reversal symmetry (TRS) and Inversion symmetry (IS) protect a Dirac node if it is pinned at zone corner X

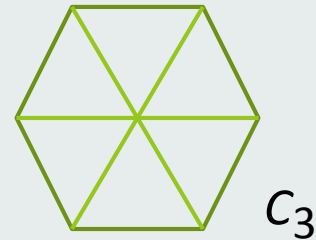
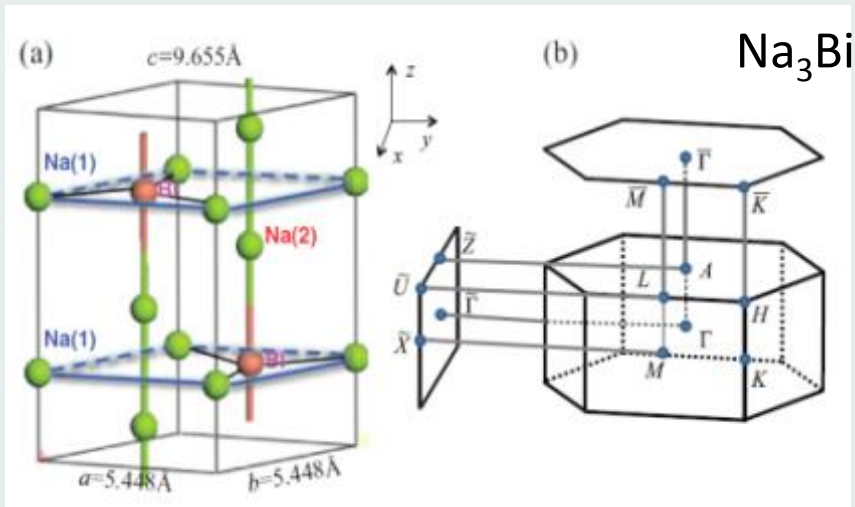
Candidate: β cristobalite BiO_2

Add point group symmetry to TRS and IS to unpin from BZ vertex

(Bernevig, XiDai, PRL 2013)

Topological Dirac semimetals Na₃Bi and Cd₃As₂

Na₃Bi and Cd₃As₂ (Wang *et al.*)



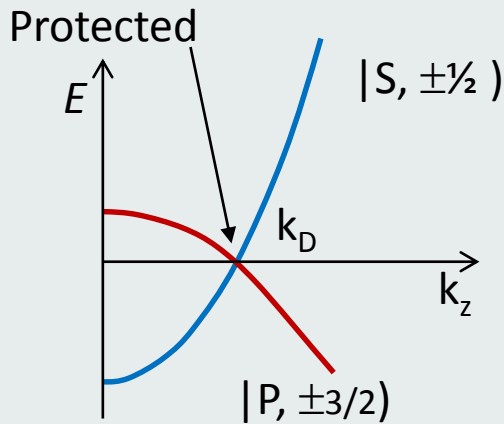
Zhijun Wang, Xi Dai et al, PRB 2012

Wan, Turner, Vishwanath, *PRB* 2011

Burkov, Hook, Balents, *PRB* 2011

Son, Spivak, *PRB* 2013

Dirac cone resolves into two Weyl nodes with opposite chiralities $\chi = \pm 1$



The low- E Hamiltonian, close to node \mathbf{K}_+ , reduces to

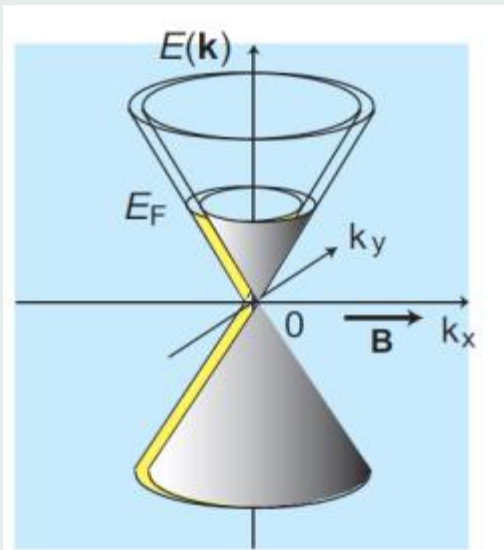
$$H = v \begin{bmatrix} k_z & k_+ & 0 & 0 \\ k_- & -k_z & 0 & 0 \\ 0 & 0 & k_z & -k_- \\ 0 & 0 & -k_+ & -k_z \end{bmatrix} \begin{pmatrix} S, 1/2 \\ P, 3/2 \\ S, -1/2 \\ P, -3/2 \end{pmatrix}$$

H resolves into two 2x2 Weyl Hamiltonians H_1, H_2

Calculate chirality from velocity matrix $\tilde{\mathbf{v}}$

$$H_1 = \mathbf{k} \cdot \tilde{\mathbf{v}}_1 \cdot \boldsymbol{\tau} = v(k_x \tau_1 - k_y \tau_2 + k_z \tau_3)$$

$$\tilde{\mathbf{v}}_1 = v \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

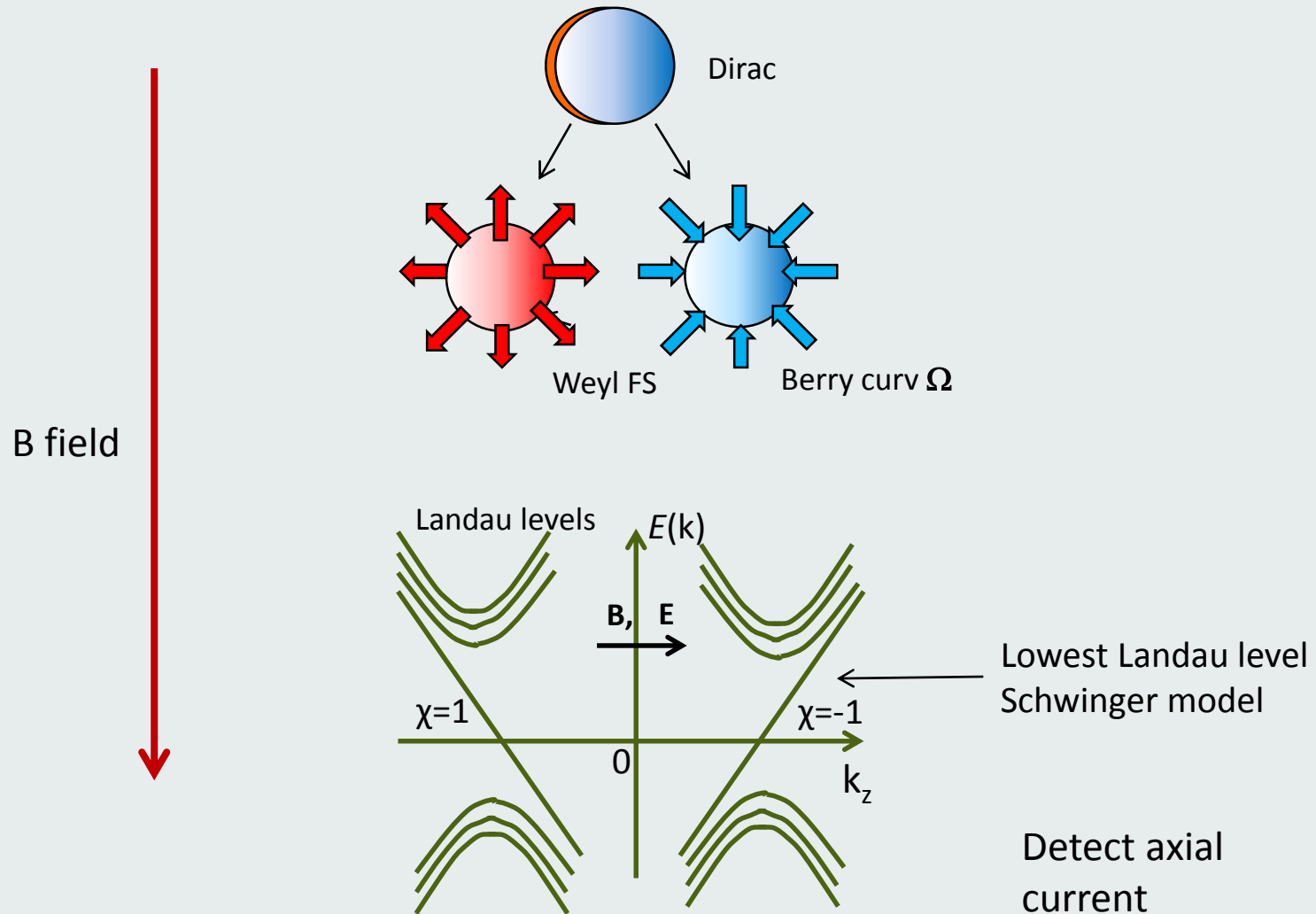


The chirality is $\chi = \frac{\det[\tilde{\mathbf{v}}]}{v}$

$$\chi_1 = -1, \quad \chi_2 = +1$$

We have a superposition of two Weyl nodes at $B = 0$

Creation of Weyl states in applied magnetic field

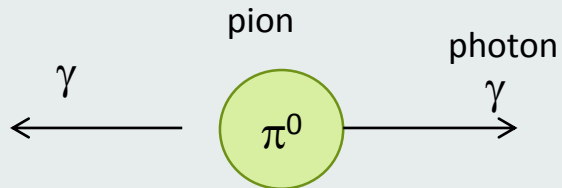


$$A = -\left(\frac{L^2}{2\pi\ell_B^2}\right)\left(\frac{Le\dot{k}_z}{2\pi}\right) = -V\frac{e^3}{4\pi^2\hbar^2}\mathbf{E}\cdot\mathbf{B}$$

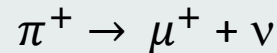
The chiral (or Adler Bell Jackiw) anomaly

An anomaly in QFT is the breaking of a classically allowed symmetry by quantum effects.

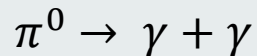
First appeared in pion decay -- discrepancy of 300 million between neutral and charged pions



Pions, the lightest hadrons, are long-lived.
Charged pions can decay only into leptons



However, *neutral* pions can decay into 2 photons (3×10^8 faster)



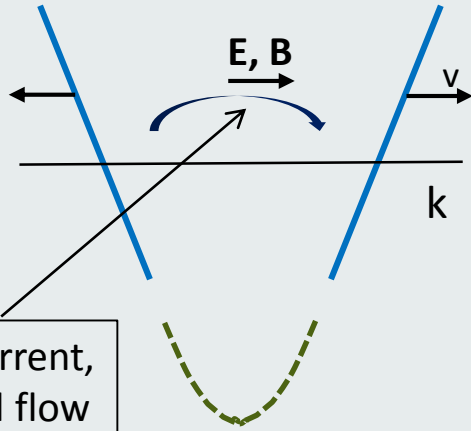
(Adler, Bell, Jackiw, 1969)¹

Coupling to EM field breaks chiral symmetry of pions
Leads to decay of axial current into photons



Adler Bell Jackiw anomaly

chiral Landau Level



Adler Bell Jackiw anomaly

$$A = \frac{1}{16\pi^2} \varepsilon^{\mu\nu\alpha\beta} \text{tr} F_{\mu\nu} F_{\alpha\beta}$$

B quantizes Dirac states into Landau levels

Rate at which charge is pumped in **E** field

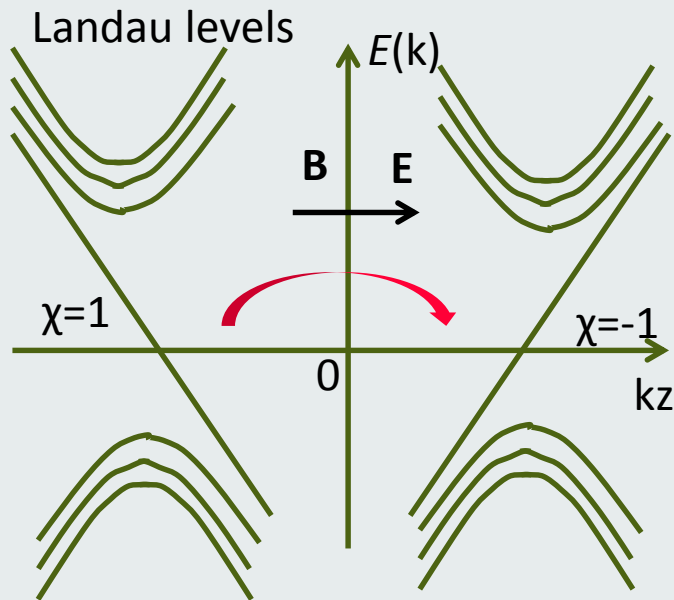
$$A = - \left(\frac{L^2}{2\pi \ell_B^2} \right) \left(\frac{Le\dot{k}_z}{2\pi} \right) = -V \frac{e^3}{4\pi^2 \hbar^2} \mathbf{E} \cdot \mathbf{B}$$

DOS of one
Landau level

Rate of increase of states
along k_z in **E** field

Chiral anomaly is observable as a large, negative longitudinal magnetoresistance (Nielsen and Ninomiya, *Phys. Lett.* 1983)

Charge pumping and the chiral anomaly



Nielsen, Ninomiya, *Phys. Lett.* 1983
 Wan, Turner, Vishwanath, *PRB* 2011
 Burkov, Hook Balents, *PRB* 2011
 Son, Spivak, *PRB* 2013
 Parameswaran et al. *PRX* 2014

Chiral anomaly engenders
 large, negative longitudinal MR
 Locked to B field

In large- B regime, with $\mathbf{E} \parallel \mathbf{B}$, charge is pumped between Weyl nodes at the rate

$$A = -\frac{L^2}{2\pi\ell_B^2} \frac{Le\dot{k}}{2\pi} = -V \frac{e^3}{4\pi^2\hbar^2} \mathbf{E} \cdot \mathbf{B}$$

In weak B , charge pumping gives (Son and Spivak, *PRB* 2013)

$$\sigma_\chi = \frac{e^2}{4\pi^2\hbar c} \frac{v}{c} \frac{(eBv)^2}{\epsilon_F^2} \tau_a$$

τ_a is relaxation time
 for pumped current

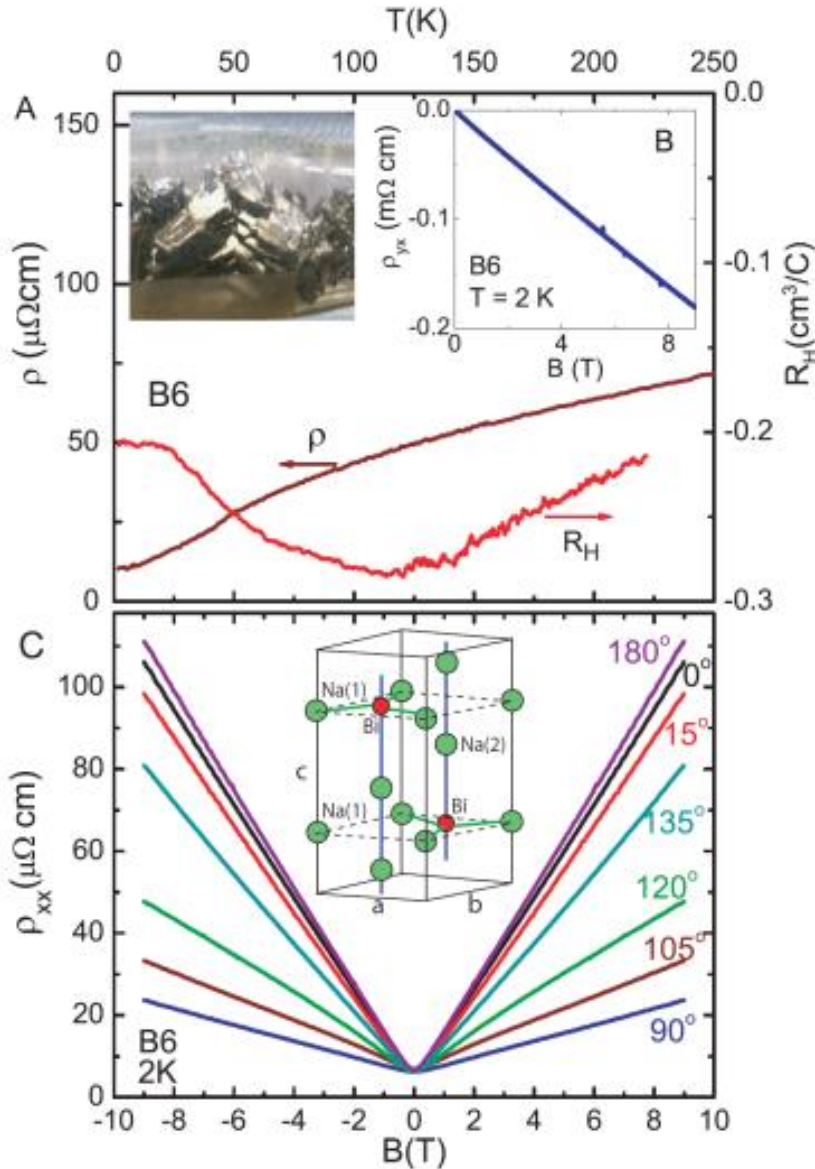
Initial results on Na₃Bi

S. Kushwaha *et al.*, APL 2015

Jun Xiong *et al.*, EPL 2015

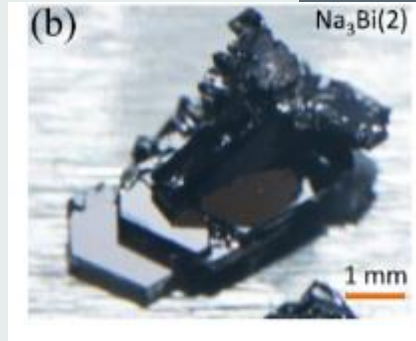


Jun Xiong Kushwaha Krizan



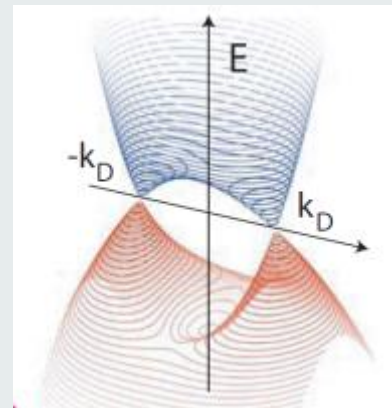
Deep purple crystals

Rapidly oxidizes in ambient air (30 s)

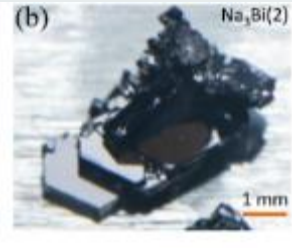


Large linear MR similar to Set B Cd₃As₂ samples

E_F 400 mV above node



Non-metallic Crystals of Na₃Bi with lower carrier density



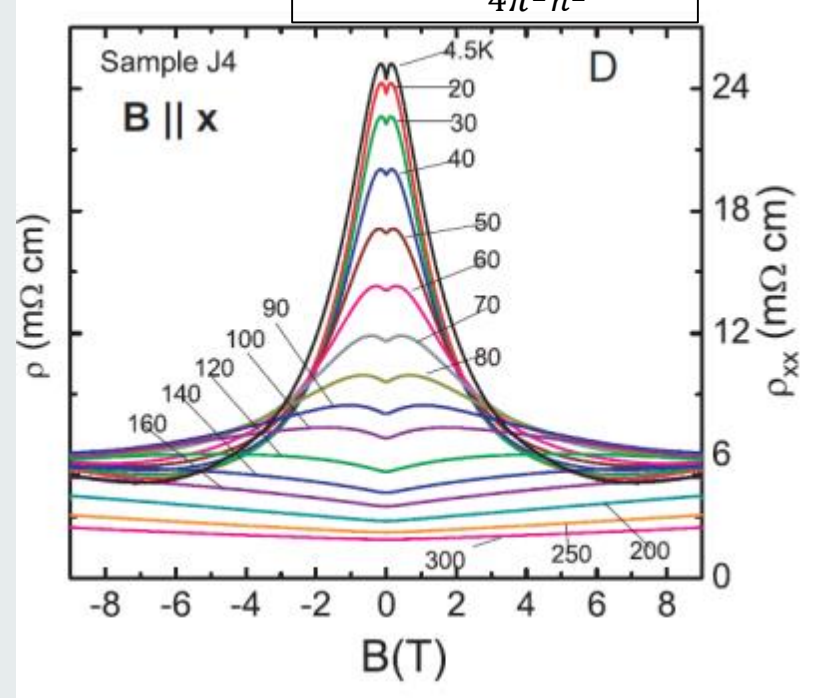
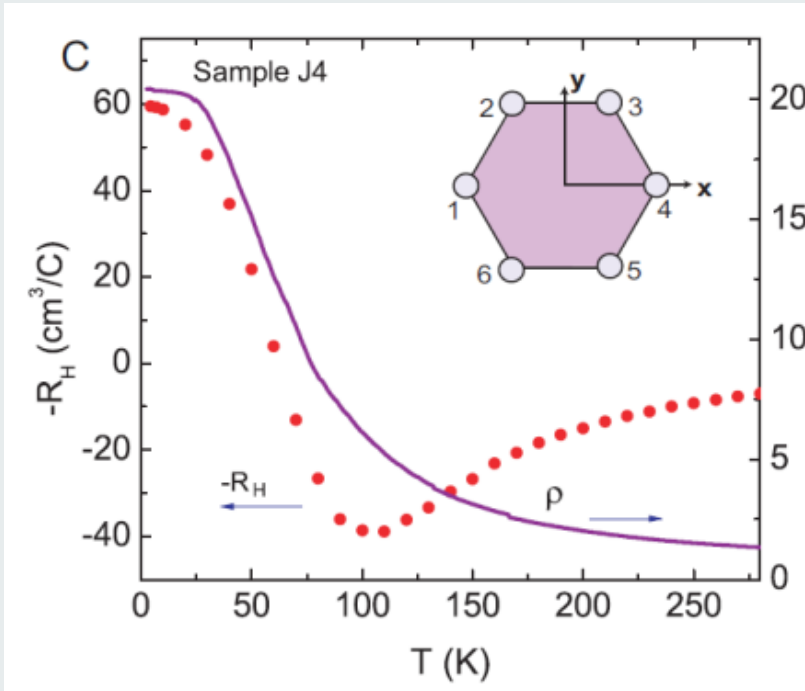
Jun Xiong, S. Kushwaha et al., *Science* 2015



Jun Xiong, S. Kushwaha, Krizan,

Long-term annealed crystals with E_F much closer to node

$$A = -V \frac{e^3}{4\pi^2 \hbar^2} \mathbf{E} \cdot \mathbf{B}$$

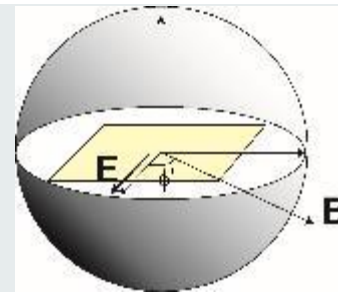
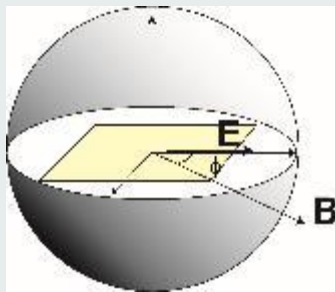
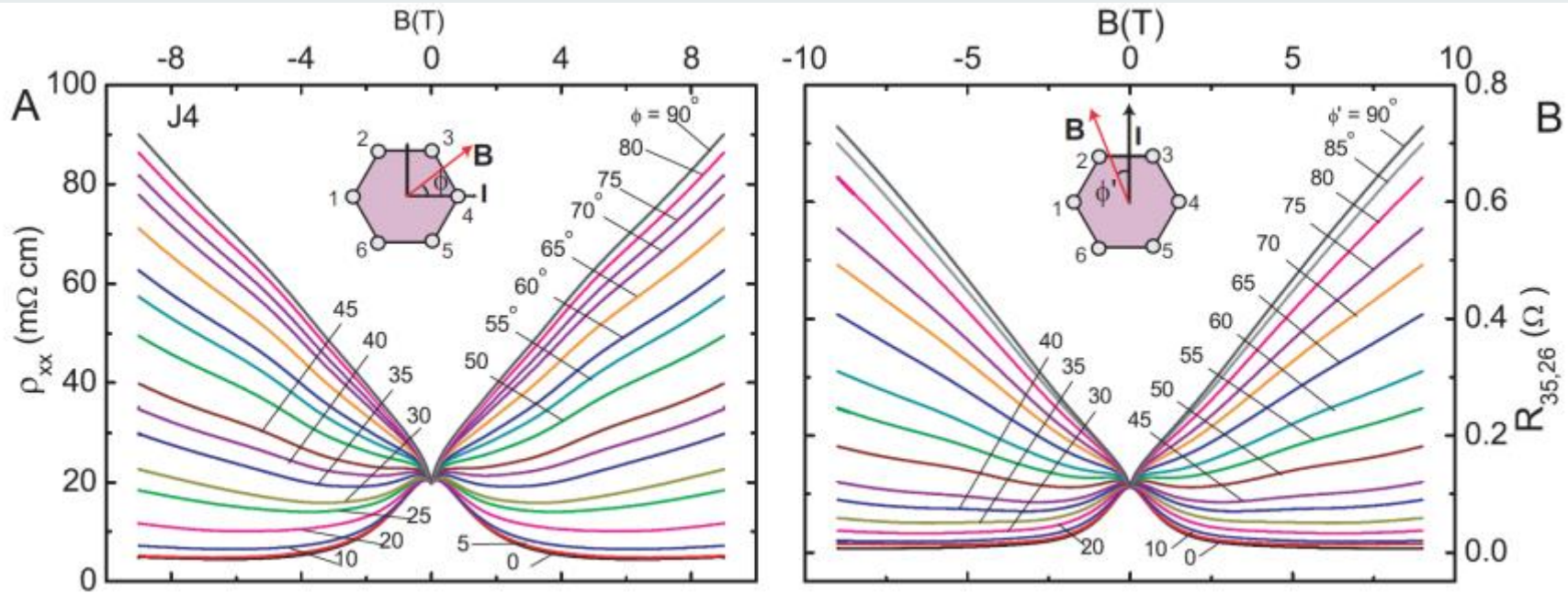


Fermi energy lies 30 meV above node

Striking negative longitud. MR (LMR)

A test for the chiral anomaly -- **B** is locked to **E**

Jun Xiong, S. Kushwaha et al., Science 2015



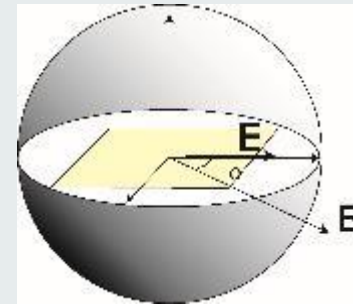
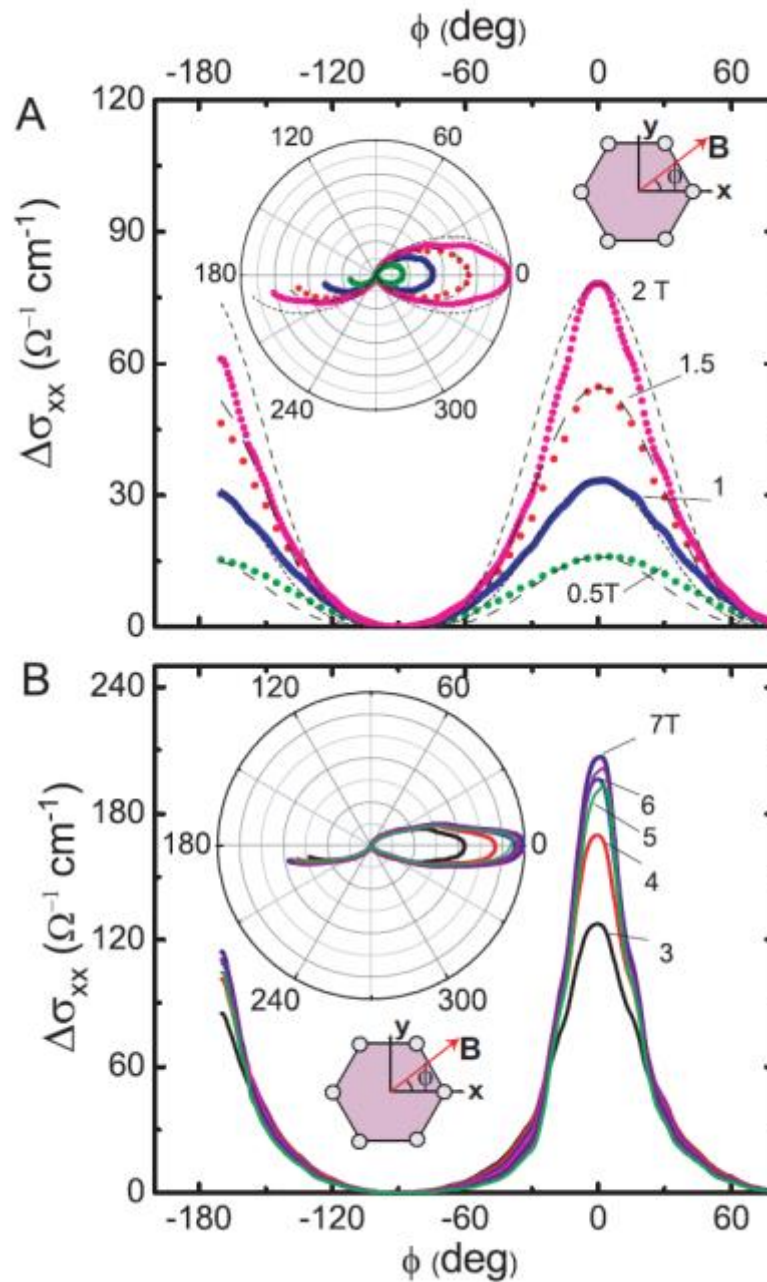
Negative MR appears only when **B** is locked to **E**.

Test: if **E** is rotated by 90° (right panel), neg. MR shifts to new direction of **E**.

For weak **B**, this locking is novel and unexpected in semiclassical transport

A narrow plume of chiral current, \mathbf{B} in-plane

Jun Xiong, S. Kushwaha et al., Science 2015



Enhanced cond. in a narrowly collimated beam for \mathbf{B} in the x - y (horizontal) plane

Chiral anomaly and thermopower of Weyl fermions in half-Heusler GdPtBi

Max Hirschberger, S. Kushwaha, ZJ Wang, Quinn Gibson, C. Belvin, B. A. Bernevig, R. J. Cava and N. P. O

Nature Materials, 2016



M. Hirschberger



S. Kushwaha



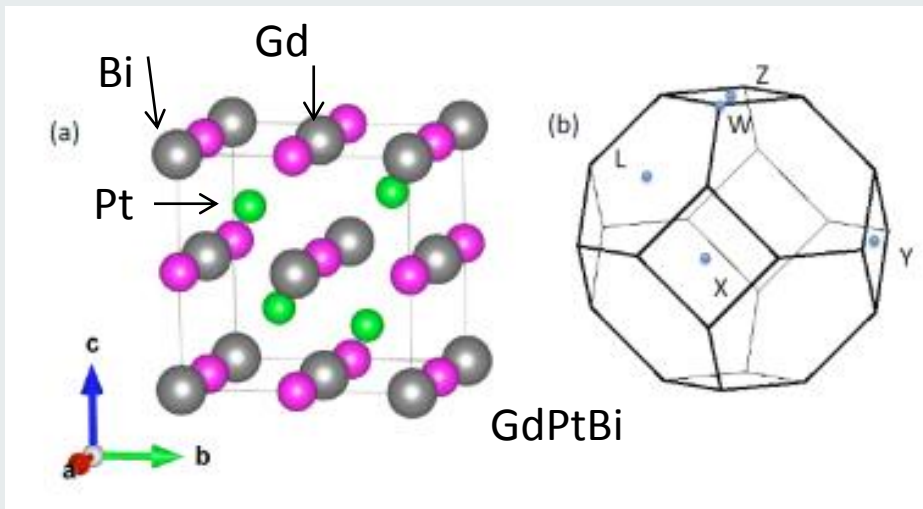
Zhijun Wang



Cano



Bradlyn



Zinc blende structure (like GaAs)

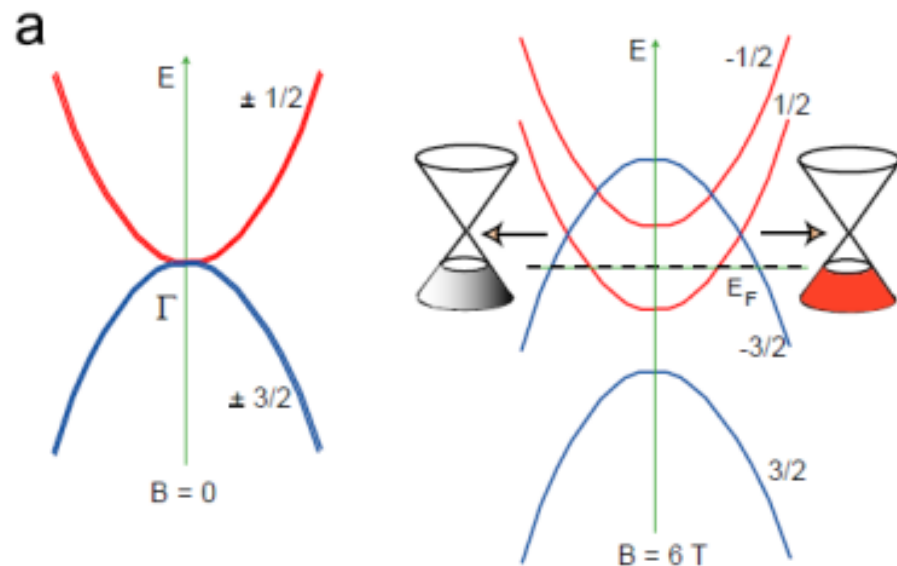
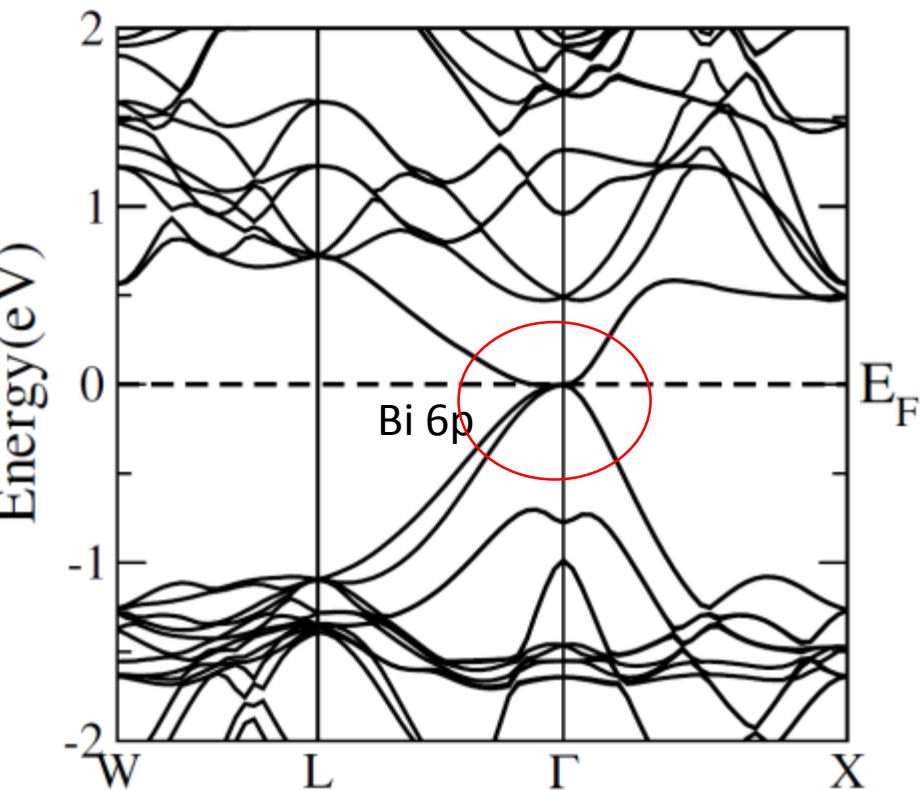
Except Bi is “stuffed” in fcc sublattice

See also, Checkelsky *Nat. Mat.* 2016
Felser, Parkin arXiv 2016

LDA calculations – effect of B on bands in GdPtBi



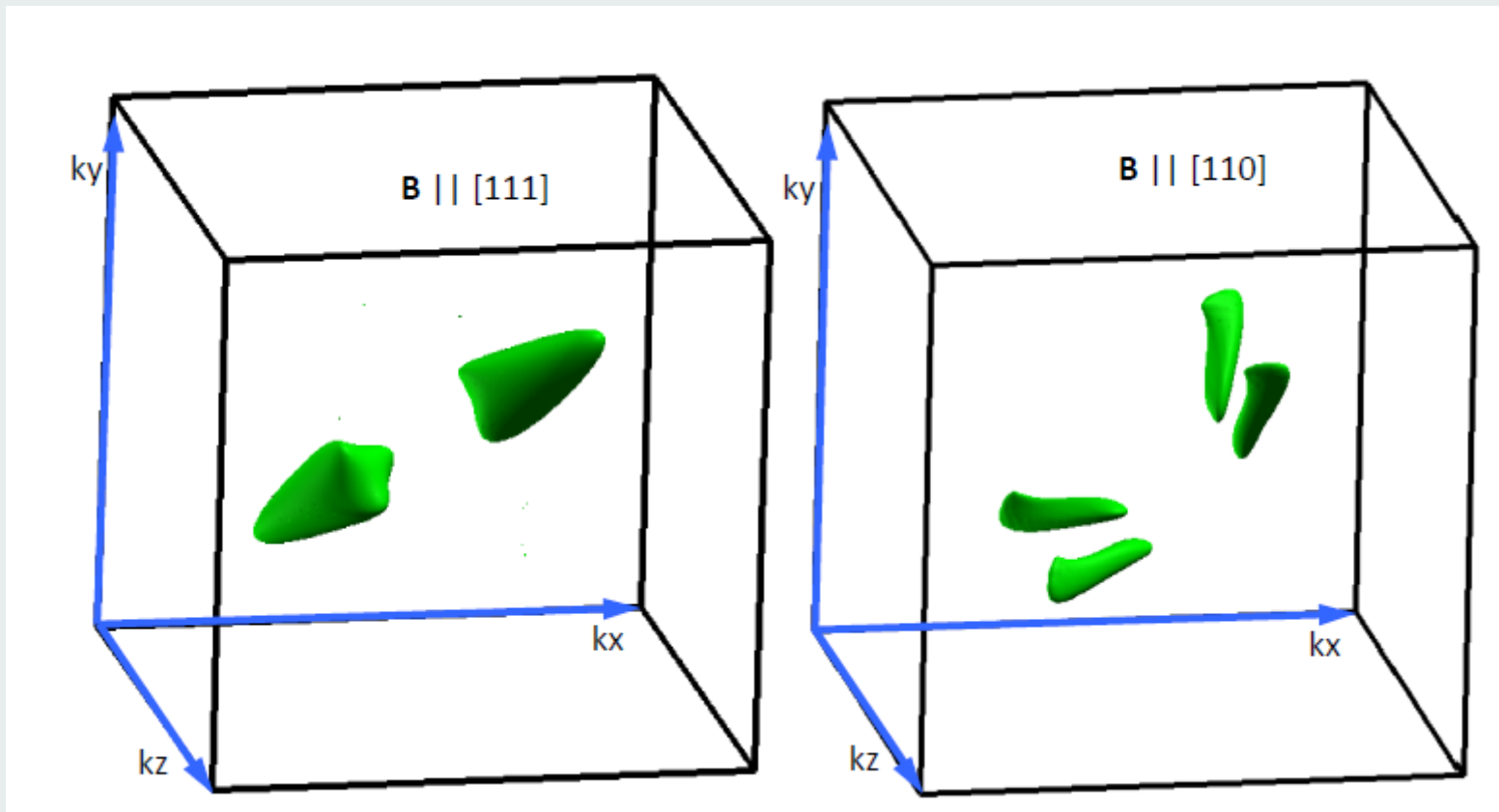
Zhijun Wang



Low-lying states (4) are derived from Bi 6p
Quadratic bands touch at Γ to form zero gap
Large spin orbit coupling

In finite B, large Zeeman field lifts degeneracies
Leads to creation of two Weyl nodes

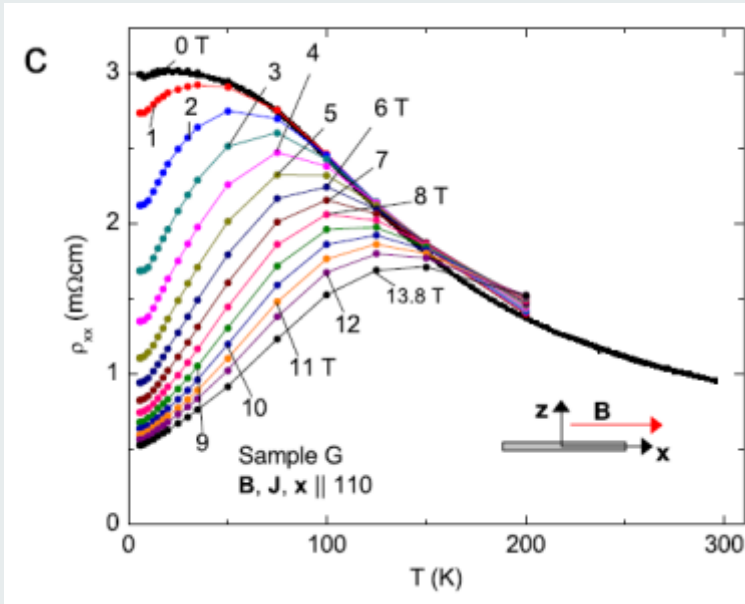
Weyl nodes created in magnetic field



Weyl nodes in a 10-Tesla B (along 111 and 110)
Derived from LDA calculations (Zhijun Wang)

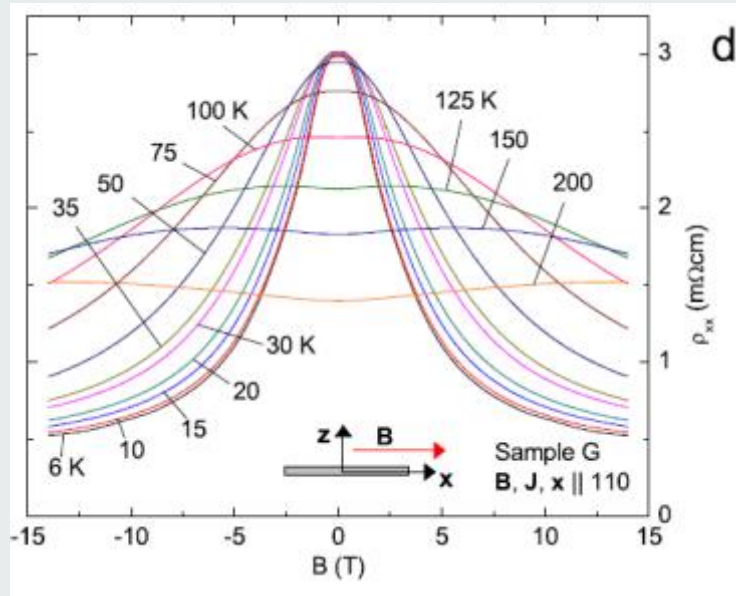
Evidence for chiral anomaly in GdPtBi

Max Hirschberger et al., Nat. Mat. 2016



Longitudinal resistivity ρ_{xx} vs. T at selected B

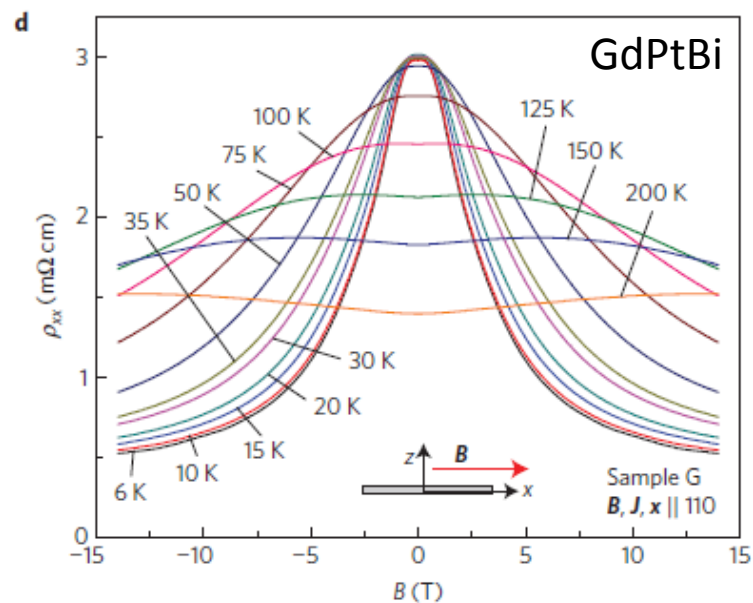
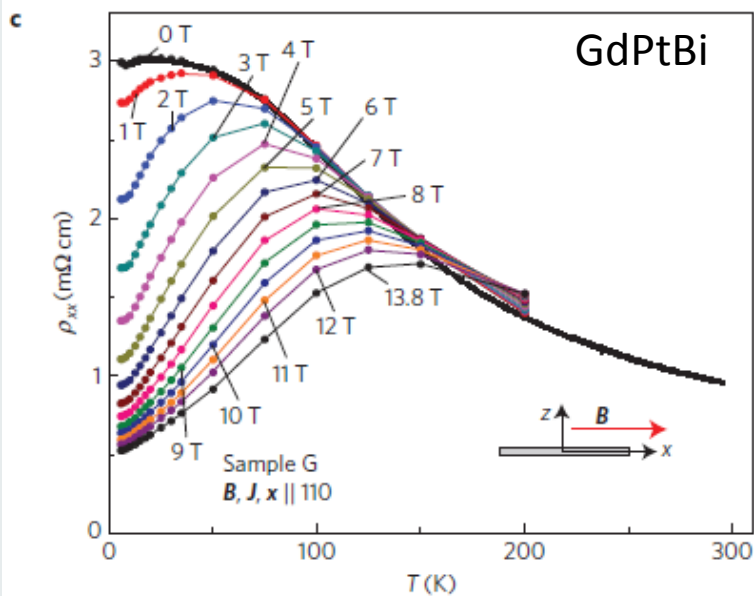
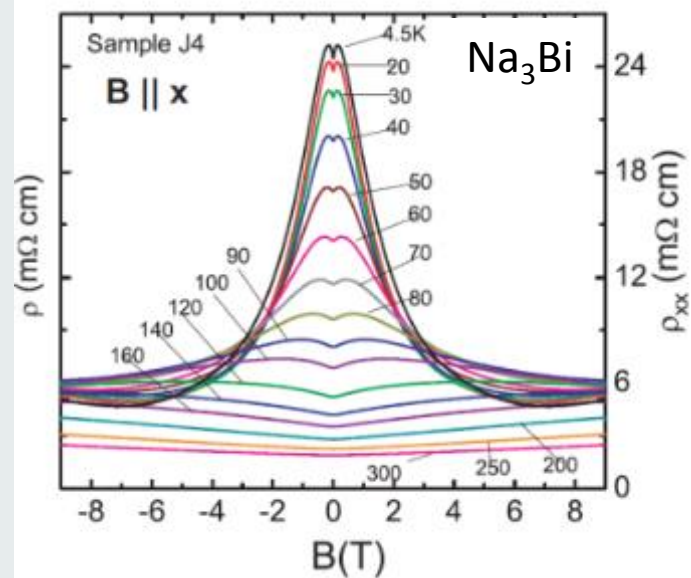
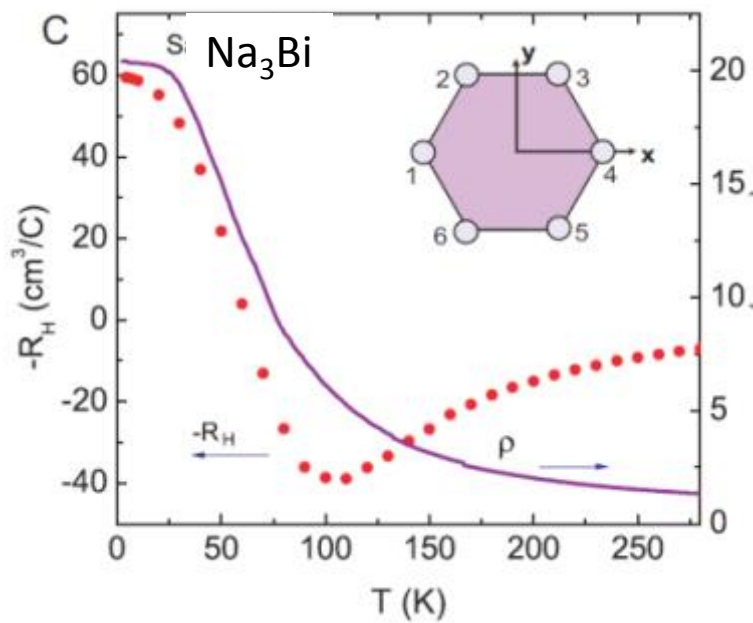
Large suppression of ρ_{xx} at low T and large B



MR profile shows large suppression of ρ_{xx} when B exceeds ~ 3 T

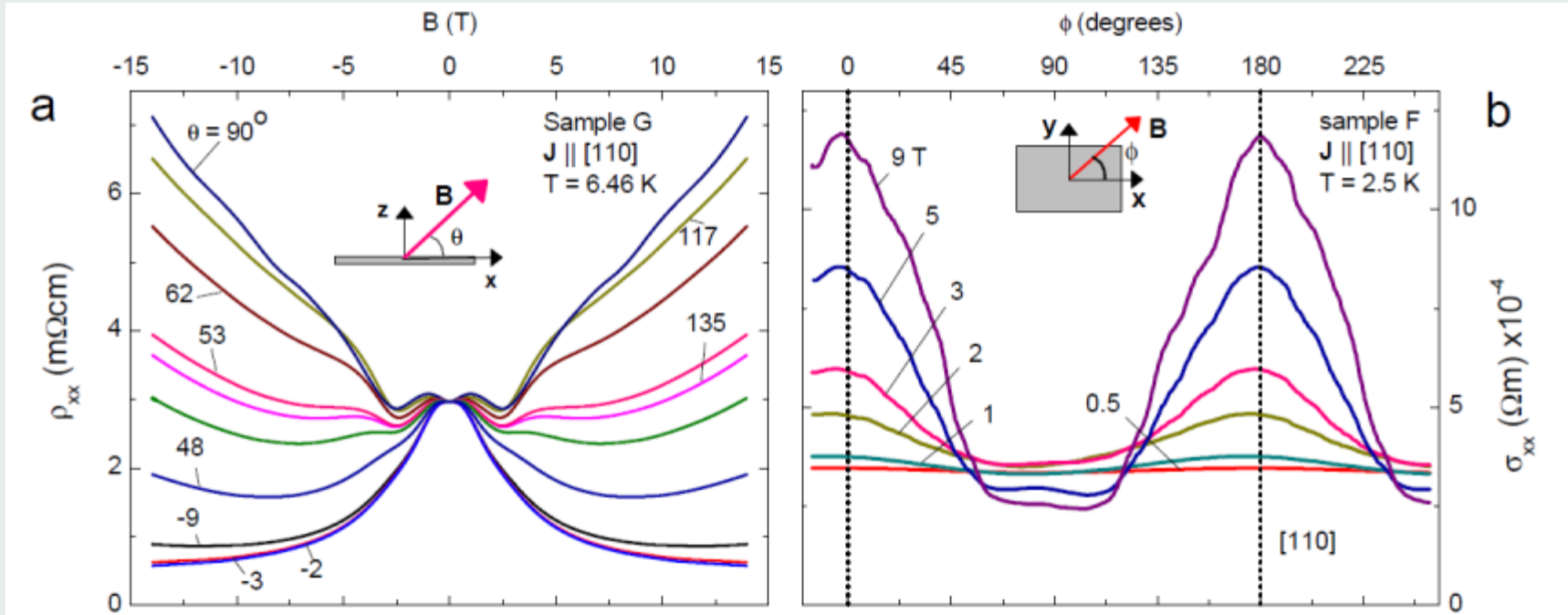
Comparison with Na_3Bi suggests existence of chiral anomaly

Resemblance between long. MR in Na₃Bi and GdPtBi



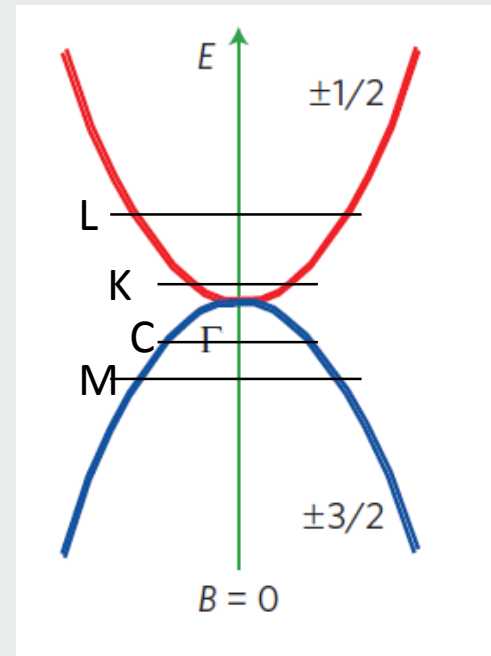
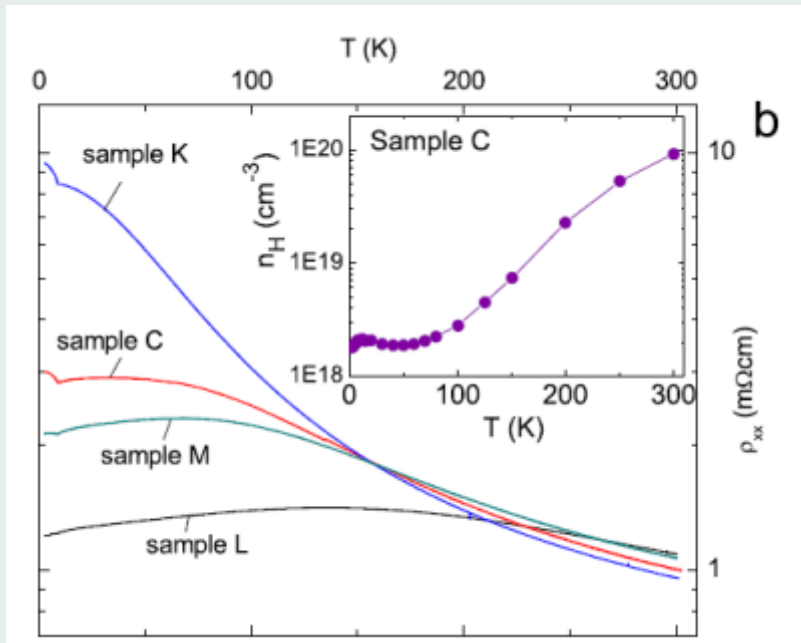
Angular dependence of current plume

Max Hirschberger et al., Nat. Mat. 2016



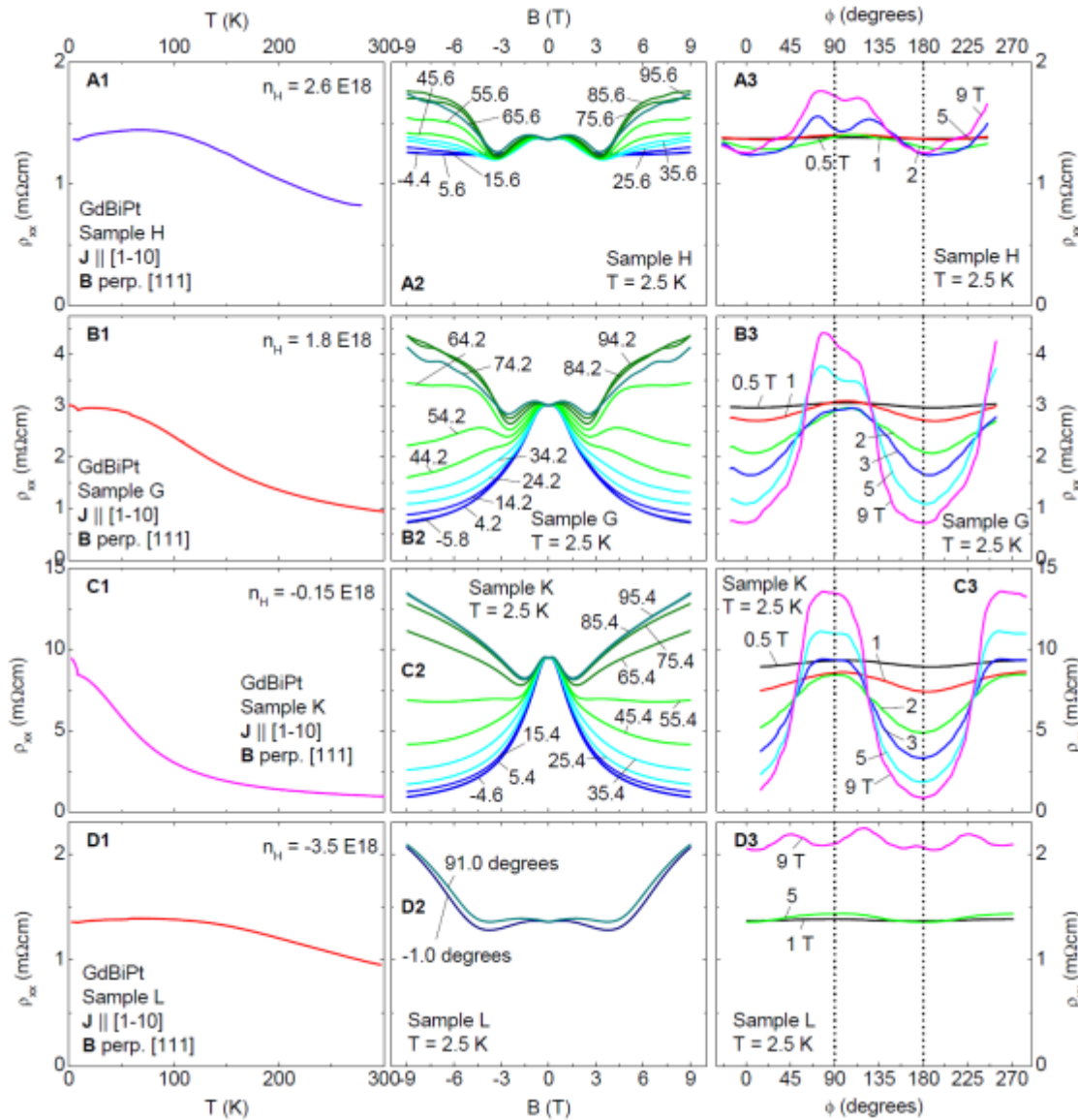
Axial current plume is largest when B approaches alignment with J

Dependence of resistivity profile on distance of E_F from node



Resistivity profiles are most non-metallic close to node

Dependence of chiral anomaly on distance of E_F from node



Maximum anomaly ampl.
when closest to node

Hole density $+2.6 \times 10^{18}$

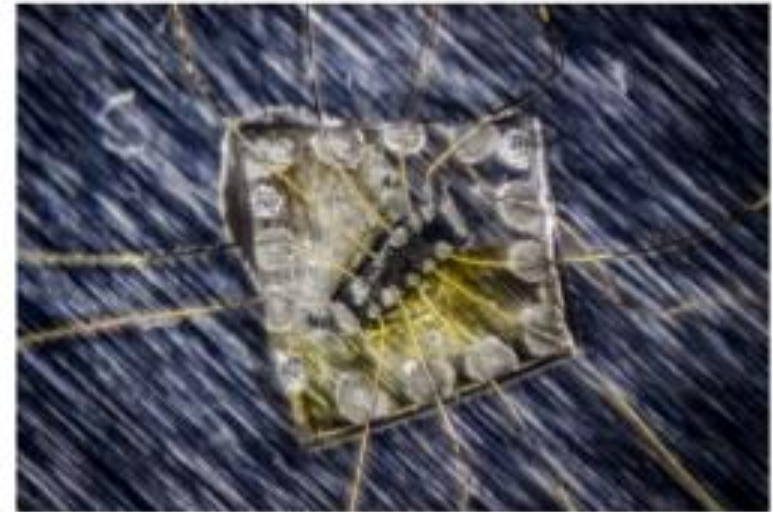
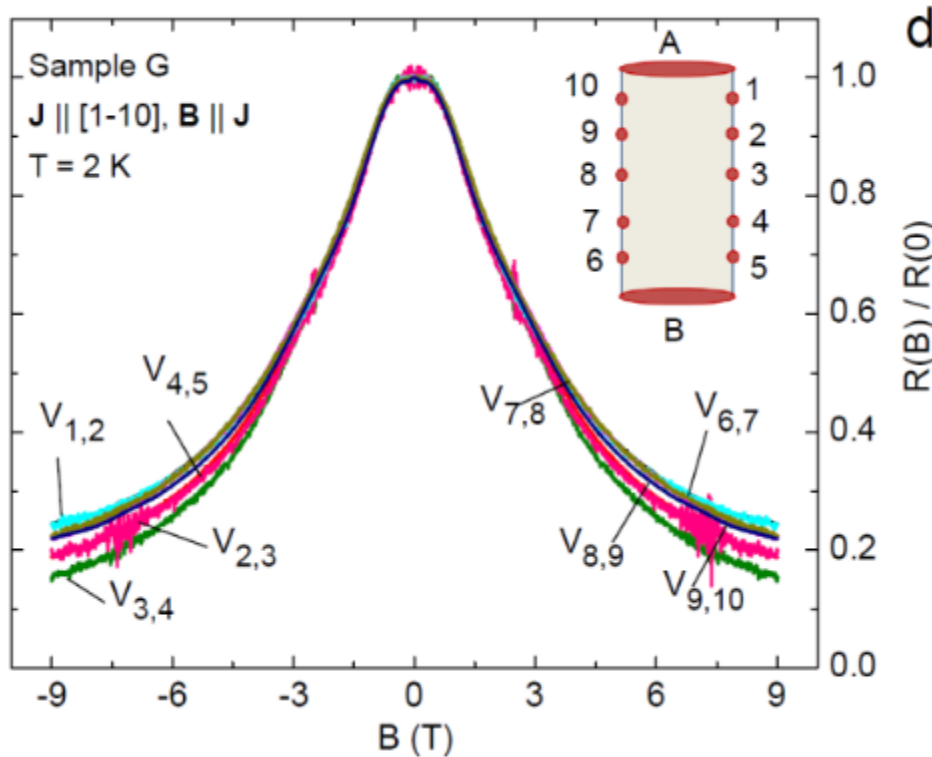
Hole density $+1.8 \times 10^{18}$

Electron density -0.15×10^{18}

Electron density -3.5×10^{18}

Check for uniformity of current density

Max Hirschberger et al., Nat. Mat. 2016



Repeat measmt. on Sample G with 10 voltage contacts

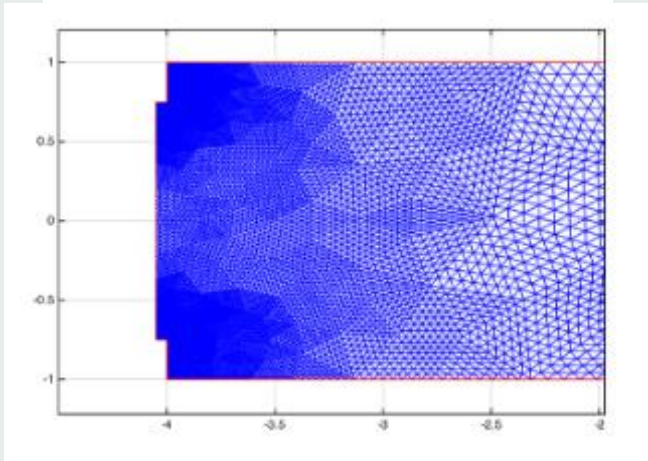
Longitud. MR profiles plotted as relative change are closely similar across all 8 nearest neighbor pairs of contacts

Conclusion: Negative longitude. MR is an intrinsic electronic effect, not a spurious result of inhomogeneity.

“Current jetting”

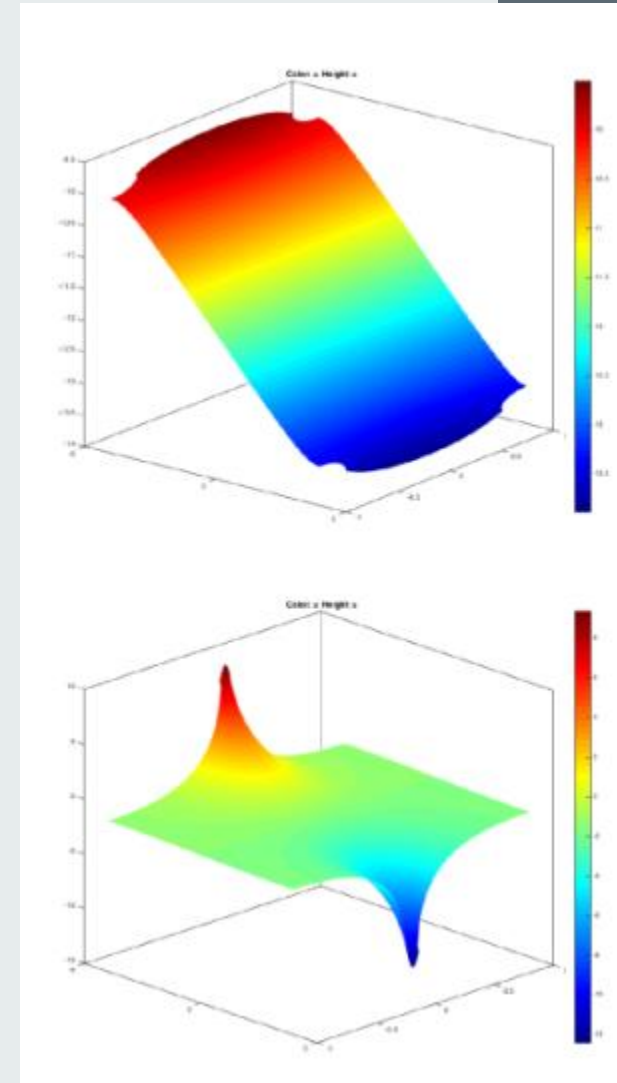
Current jetting can produce spurious, negative longitudinal MR but only in high mobility samples in intense B ($\mu B \gg 1$)

$$[\partial_x \sigma_{xx} \partial_x + \partial_y \sigma_{yy} \partial_y] \psi(x, y) = 0.$$



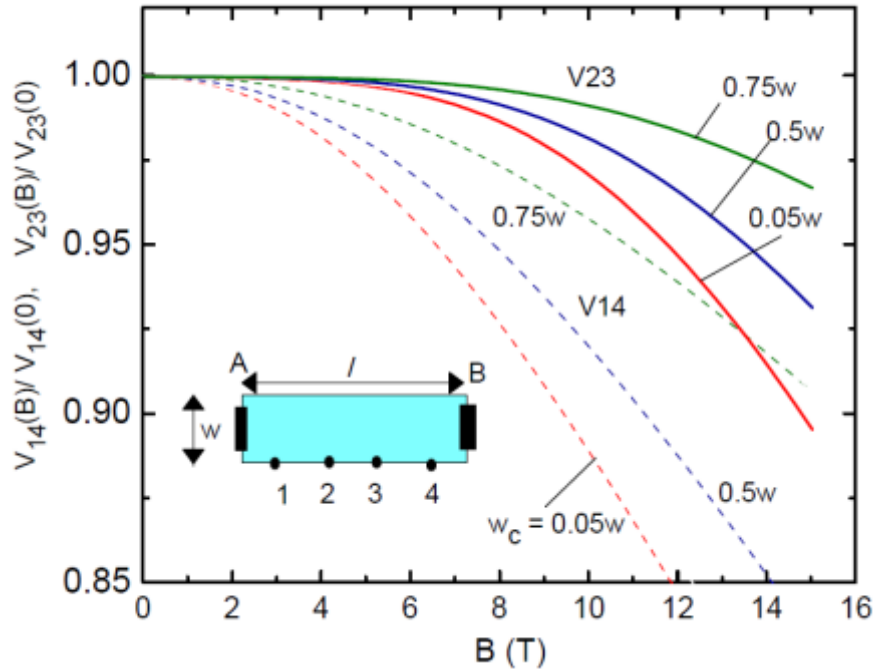
Numerically calculate potential function $\psi(x, y)$ with Drude conductivity tensor in $\mathbf{B} \parallel \mathbf{E}$.

Current jetting is unimportant for small μB and broad current contacts (upper panel). However, for point contacts and large μB (lower panel), get current focusing and jetting (imitates very large contact resistance).



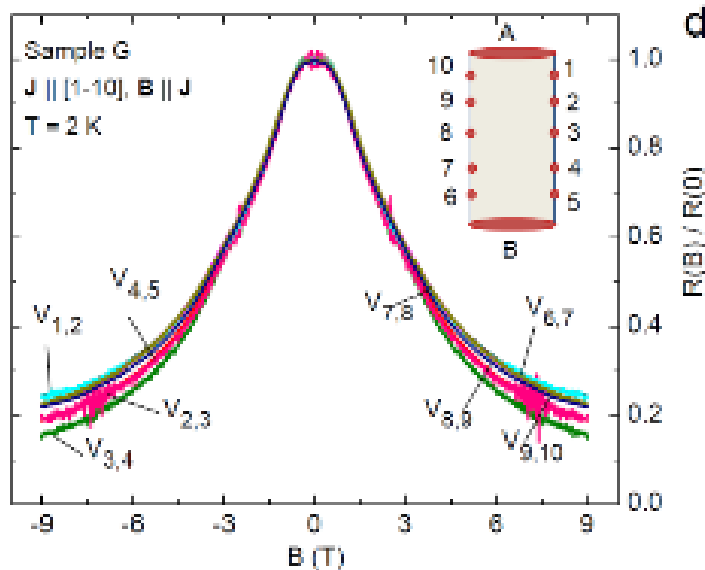
The case against “current jetting” in GdPtBi

Max Hirschberger et al., Nat. Mat. 2016



Upper panel:
Calculated $V_{ij}(B)$ curves using “current jetting” assumptions for mobility of $2,000 \text{ cm}^2/\text{Vs}$ and various current contact widths.

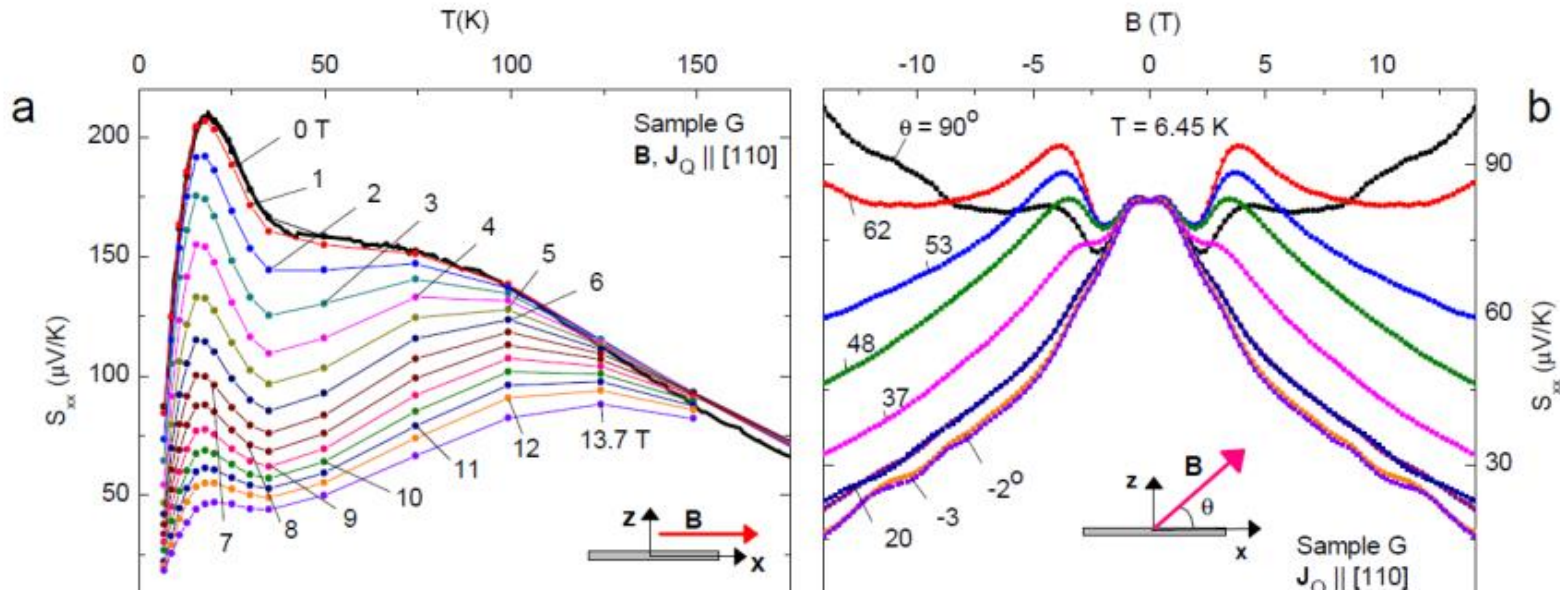
To reproduce observed long. MR curves (lower panel) we would need B to exceed 50 to 70 Tesla.



Conclusion: Current jetting is not the origin of observed chiral anomaly.

Thermopower of Weyl fermions in GdPtBi

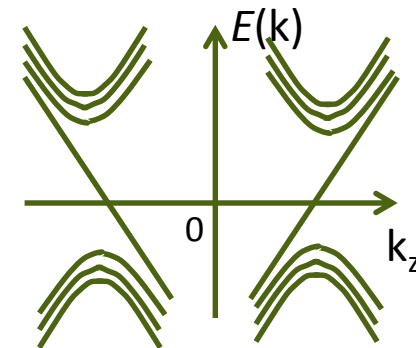
Max Hirschberger et al., Nat. Mat. 2016

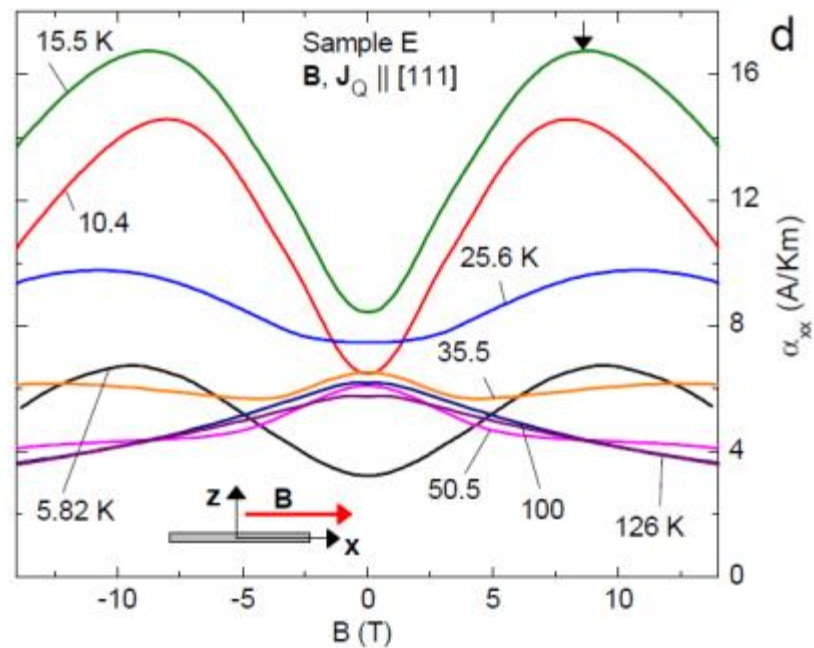
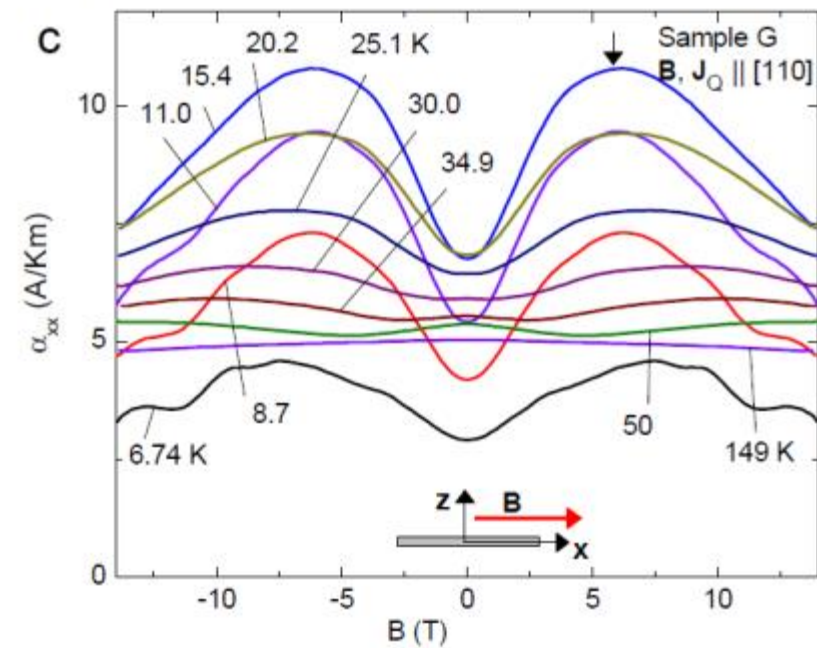
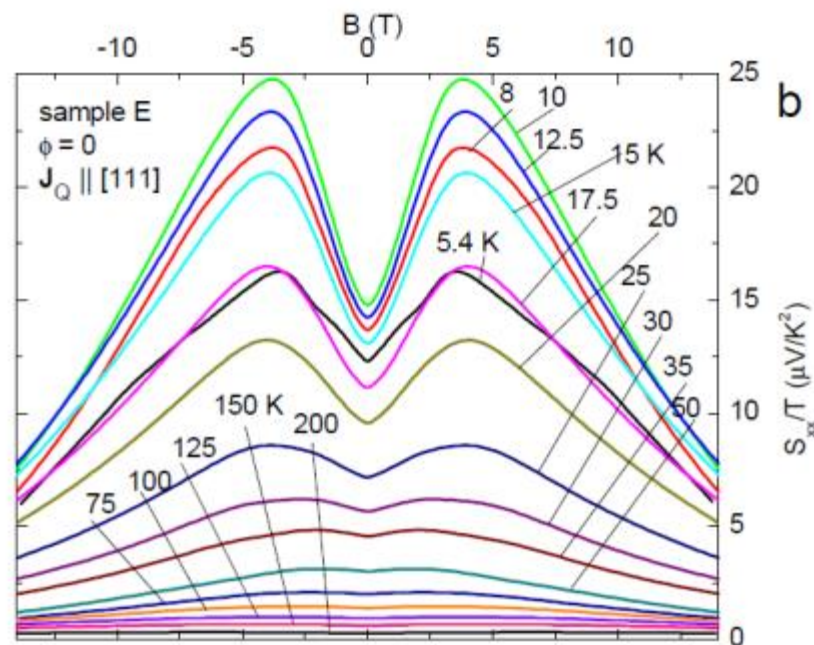
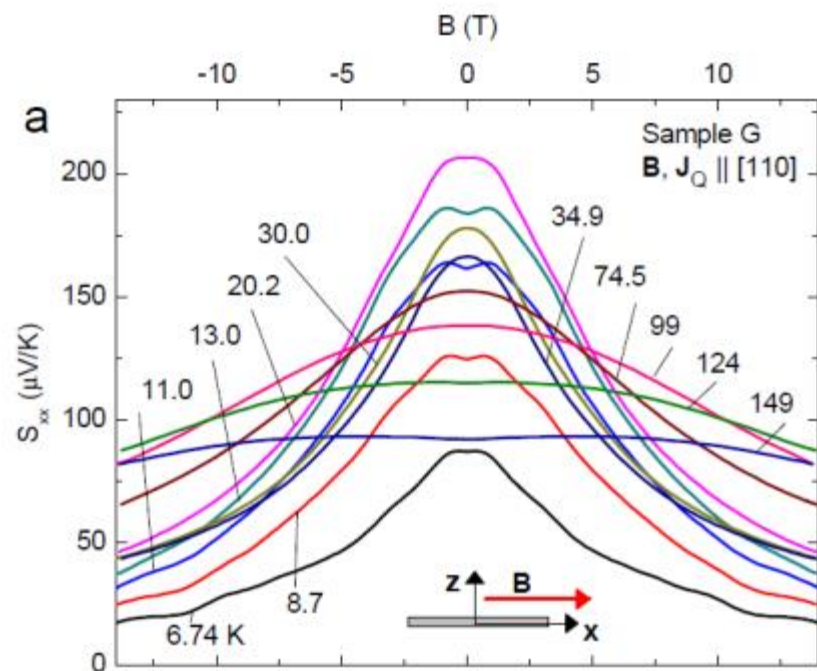


Thermoelectric response is strongly suppressed when axial current appears.

A consequence of chiral $n=0$ Landau level?

Reflects the “flat” DOS vs. E in the lowest Landau level



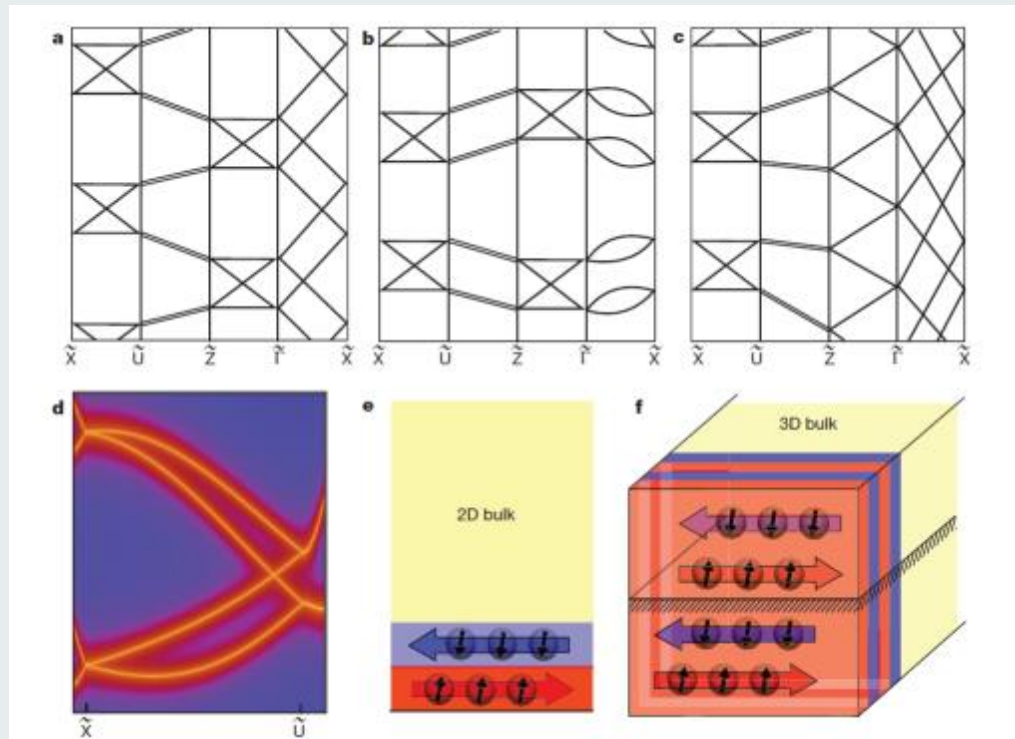
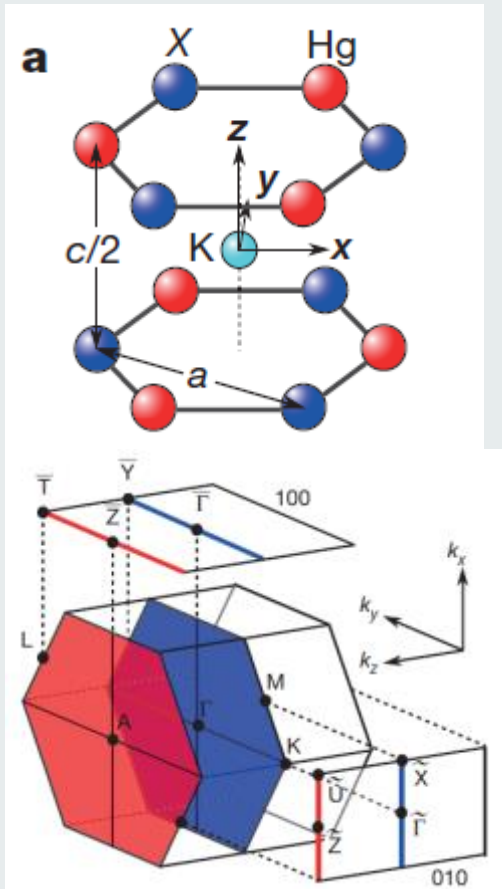


Hourglass fermions

ZJ Wang et al., *Nature* (2016)

Zhijun Wang^{1*}, A. Alexandradinata^{1,2*}, R. J. Cava³ & B. Andrei Bernevig¹

KHgSb, KHgAs



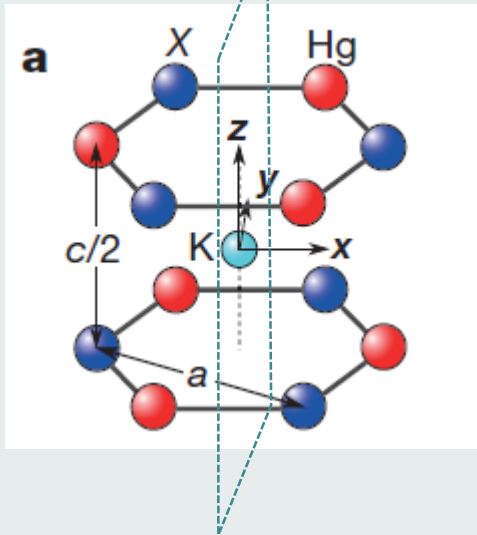
Nonsymmorphic

Two pairs of helical states wrap around sides

Hourglass fermions exist on Z - $\bar{\Gamma}$ face

Nonsymmorphic group and protected bands on BZ surface

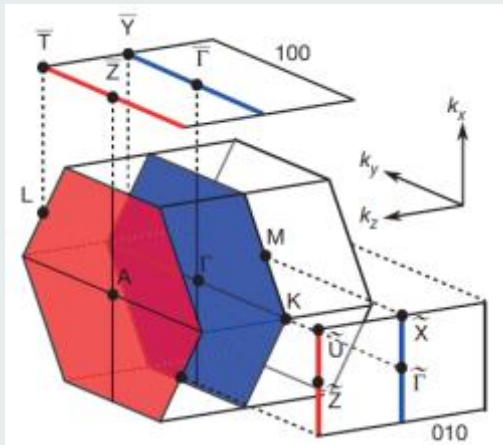
Nonsymm space groups include glide planes and screw oper.



Mirror reflection in yz plane $M_x = -i\sigma_1 P$
is not a symm operation of the group

Need to combine with translation by $\tau = \mathbf{c}/2$
 $t(\boldsymbol{\tau}) = \exp(i\mathbf{k} \cdot \boldsymbol{\tau})$

$$\overline{M}_x = t_z \left(\frac{c}{2} \right) M_x = \exp(i\mathbf{k} \cdot \frac{\mathbf{c}}{2}) (-i\sigma_1 P)$$



$$\Theta^2 \overline{M}_x^2 = \exp(ik_z c)$$

Protects pair of degenerate states on
plane $k_z = \pi/c$

SdH oscillations in KHgSb

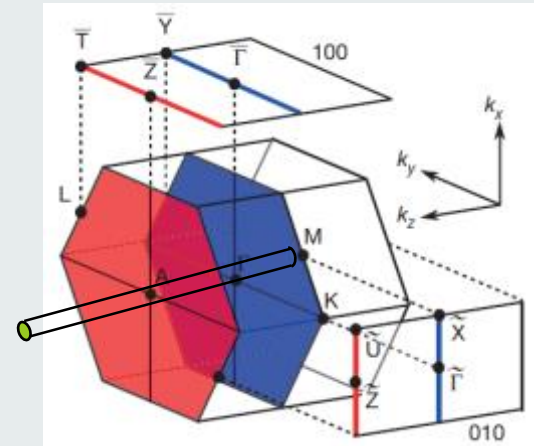
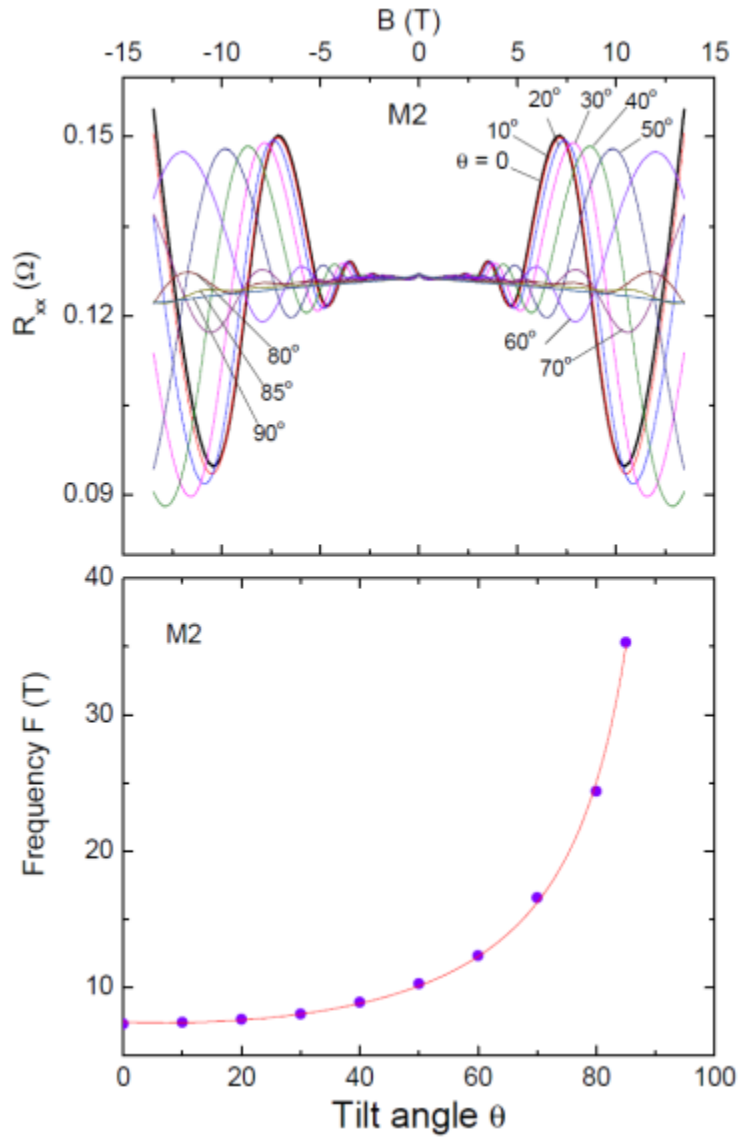
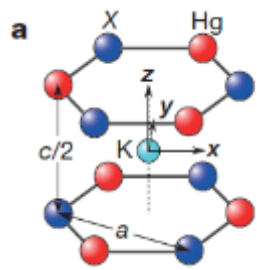
S.H. Liang et al., unpublished



S.H. Liang

S. Kushwaha

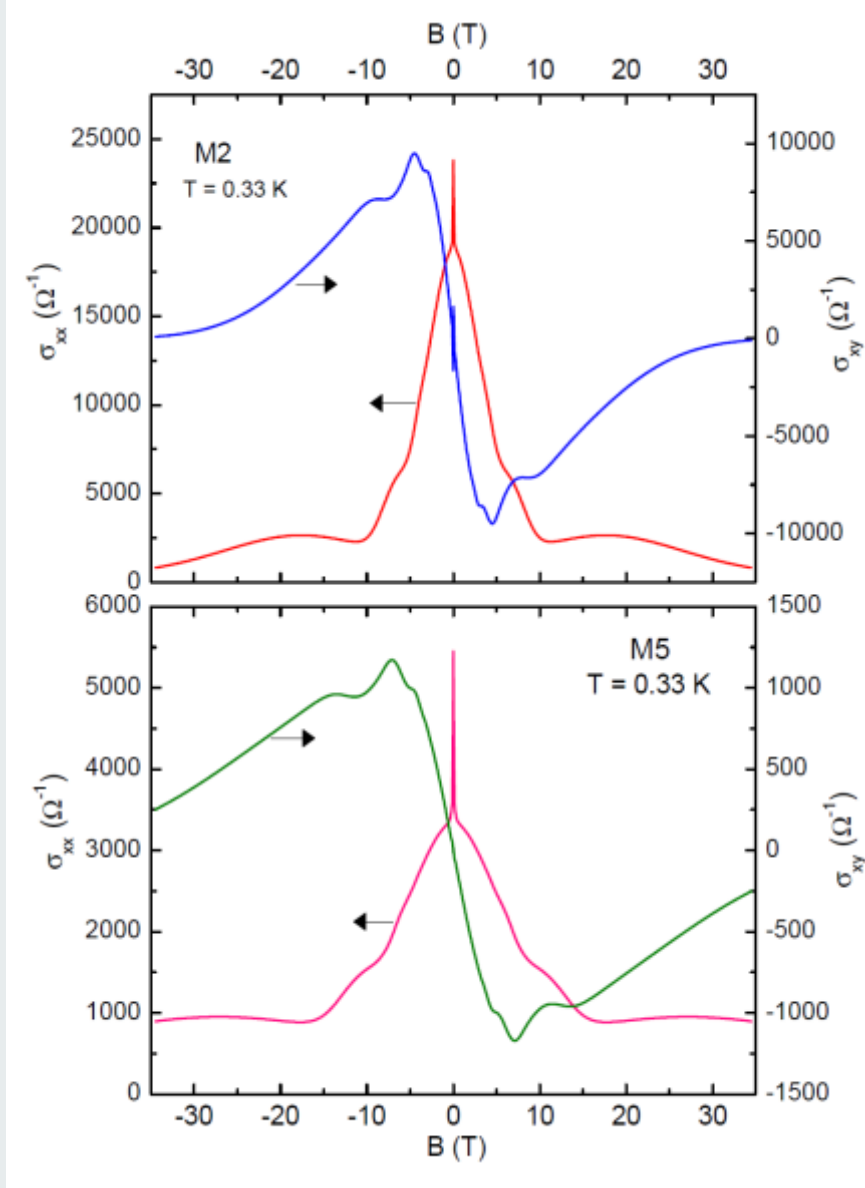
Zhijun Wang

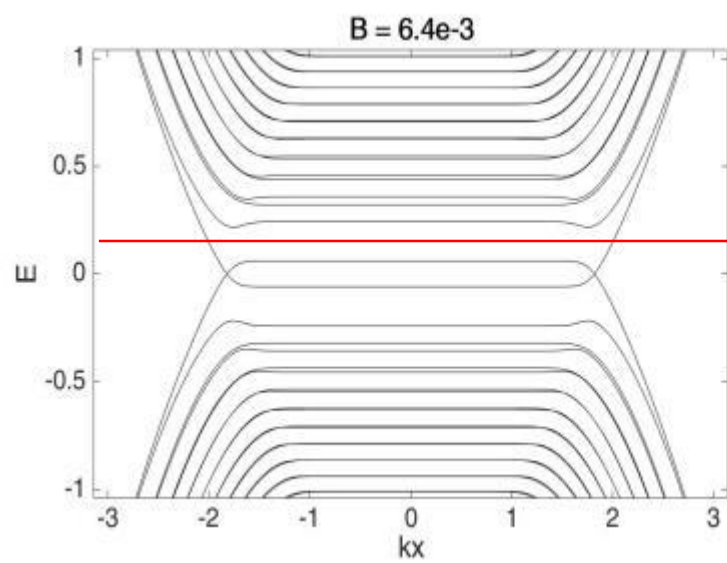
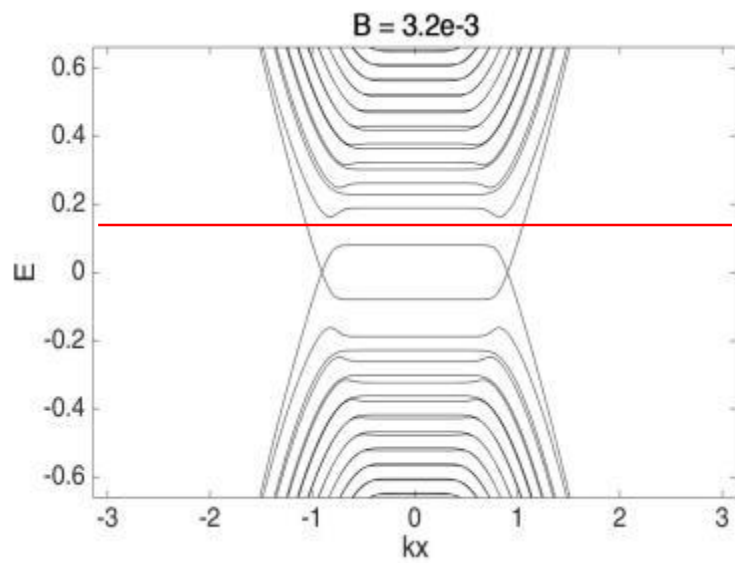
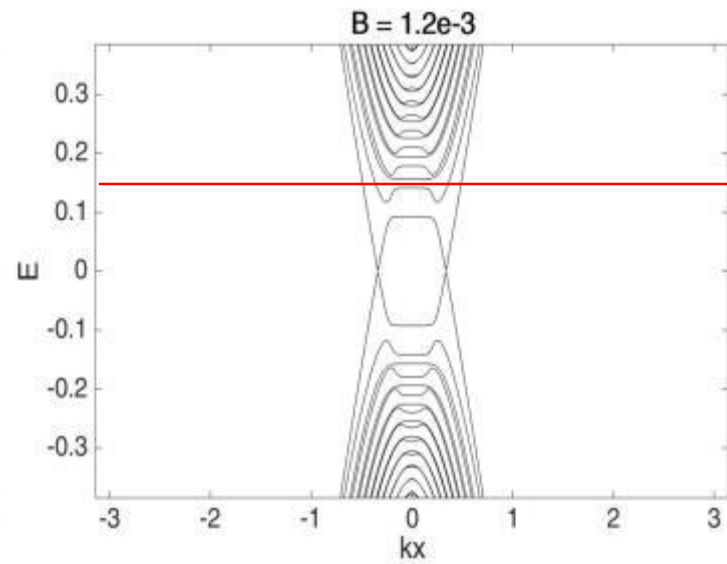
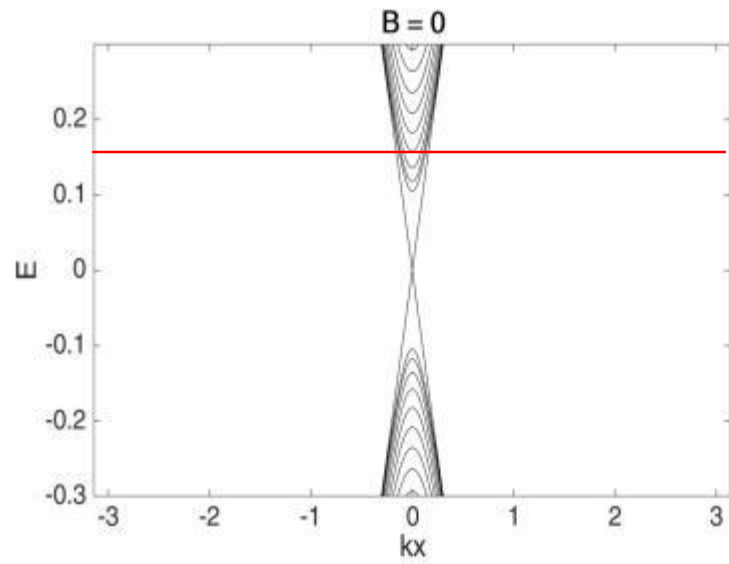


n-type carriers
occupy a narrow
FS cylinder

Abrupt change of conductivity in quantum limit

S.H. Liang et al., unpublished





Summary

- 1) Evidence for chiral anomaly in Dirac semimetal Na_3Bi
- 2) Chiral anomaly in a zero-gap semiconductor, half Heusler GdPtBi
Zeeman field induces band crossing and protected nodes
Chiral anomaly has strong effect on thermoelectric current
- 3) Nonsymmorphic semimetal KHgSb – new mode in quantum limit



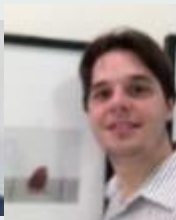
Jun Xiong



Kushwaha



Tian Liang



Jason Krizan



Hirschberger



Zhijun Wang



Quinn Gibson



Cano



Bradlyn



S.H. Liang



Bob Cava



Bernevig



NPO

Thank you

