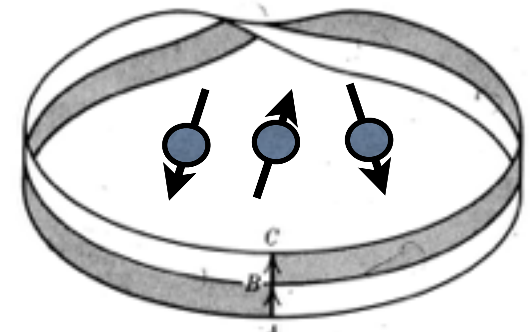
Topological Kondo Insulators:

Magnetism meets Topology



Novel Theories & Novel Materials, ICTP Trieste
11 Aug, 2015.

Piers Coleman
Center for Materials Theory, Rutgers U, USA
Hubbard Theory Consortium & Royal Holloway, University of London, UK.

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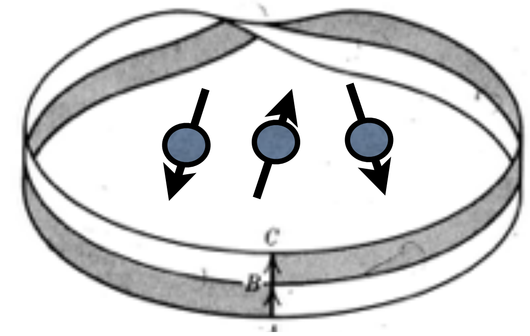

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Collaborators

Maxim Dzero	Kent State
Kai Sun	Michigan
Victor Galitski	Maryland
Vic Alexandrov,	IAS
Onur Erten,	Rutgers

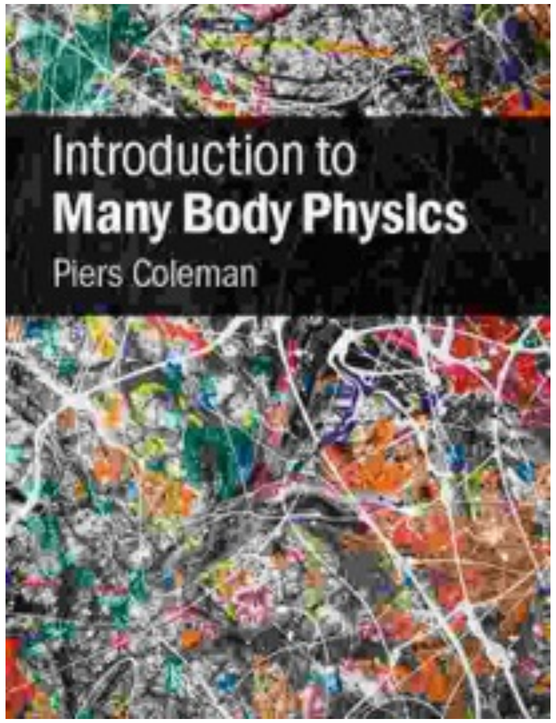
Kai Maxim Victor Vic Onur

Joel Moore,	Berkeley
Phil Anderson,	Princeton
Suchitra Sebastian	Cambridge
Gil Lonzarich	Cambridge

M. Dzero, K. Sun, V. Galitski, PC Phys. Rev. Lett. **104**, 106408 (2010)
T. Takimoto, J. Phys. Soc. Jpn. **80**, 123710 (2011).
V. Alexandrov, P. Coleman, O. Erten, Phys. Rev. Lett. 114:177202 (2015).
Maxim Dzero, Jing Xia, Victor Galitski, Piers Coleman, ***Annual Reviews CMP*** (2016), ArXiv 1506.05635

Notes:

"Introduction to Many Body Physics", Ch 8,15-16", PC, CUP (Nov. 2015).



"Heavy Fermions: electrons at the edge of magnetism." Wiley encyclopedia of magnetism. PC. cond-mat/0612006.

"I2CAM-FAPERJ Lectures on Heavy Fermion Physics", (X=I, II, III)

http://physics.rutgers.edu/~coleman/talks/RIO13_X.pdf

M. Dzero, K. Sun, V. Galitski, PC Phys. Rev. Lett. **104**, 106408 (2010)

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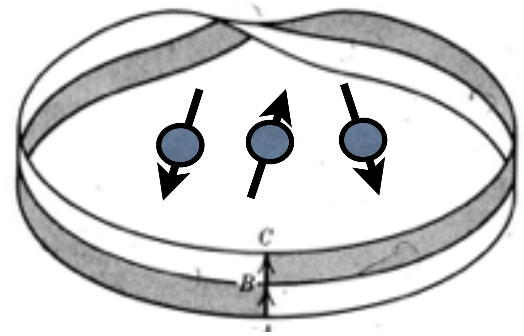


Piers Coleman & Onur Erten
Center for Materials Theory, Rutgers U, USA
Royal Holloway, University of London, UK.

Outline

- SmB_6 and the rise of topology
- TKIs: a link with superfluid He-3
- Is SmB_6 topological?
- The Magnetic Connection.

Kondo insulators: History

Menth, Buehler and Geballe (PRL 22,295, 1969)
Aeppli and Fisk (Comments CMP 16, 155, 1992)

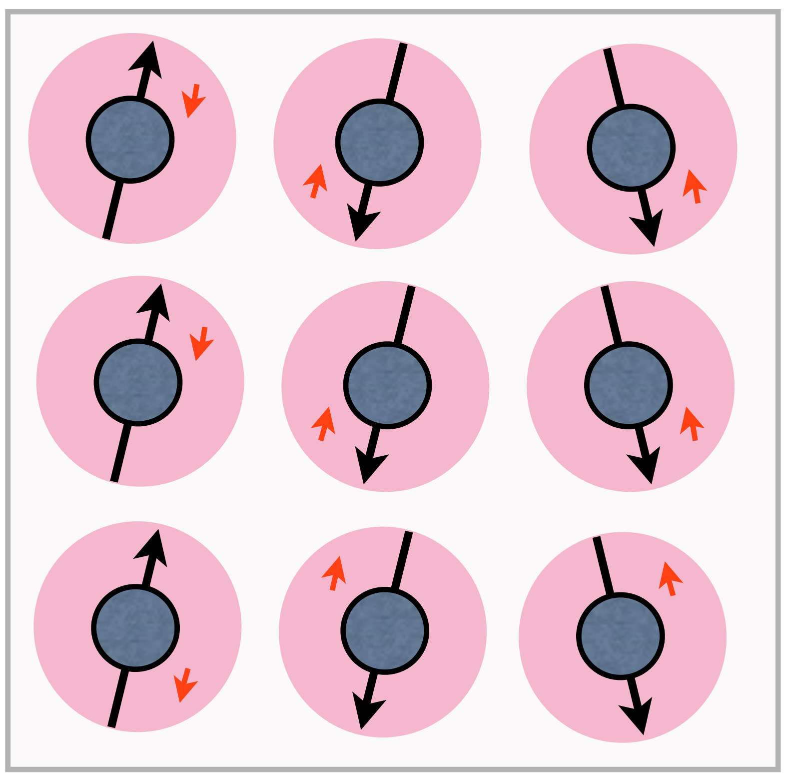
MAGNETIC AND SEMICONDUCTING PROPERTIES OF SmB_6†

A. Menth and E. Buehler
Bell Telephone Laboratories, Murray Hill, New Jersey

and

T. H. Geballe
Department of Applied Physics, Stanford University, Stanford, California,
and Bell Telephone Laboratories, Murray Hill, New Jersey
(Received 21 November 1968)

Simplest Kondo Lattice



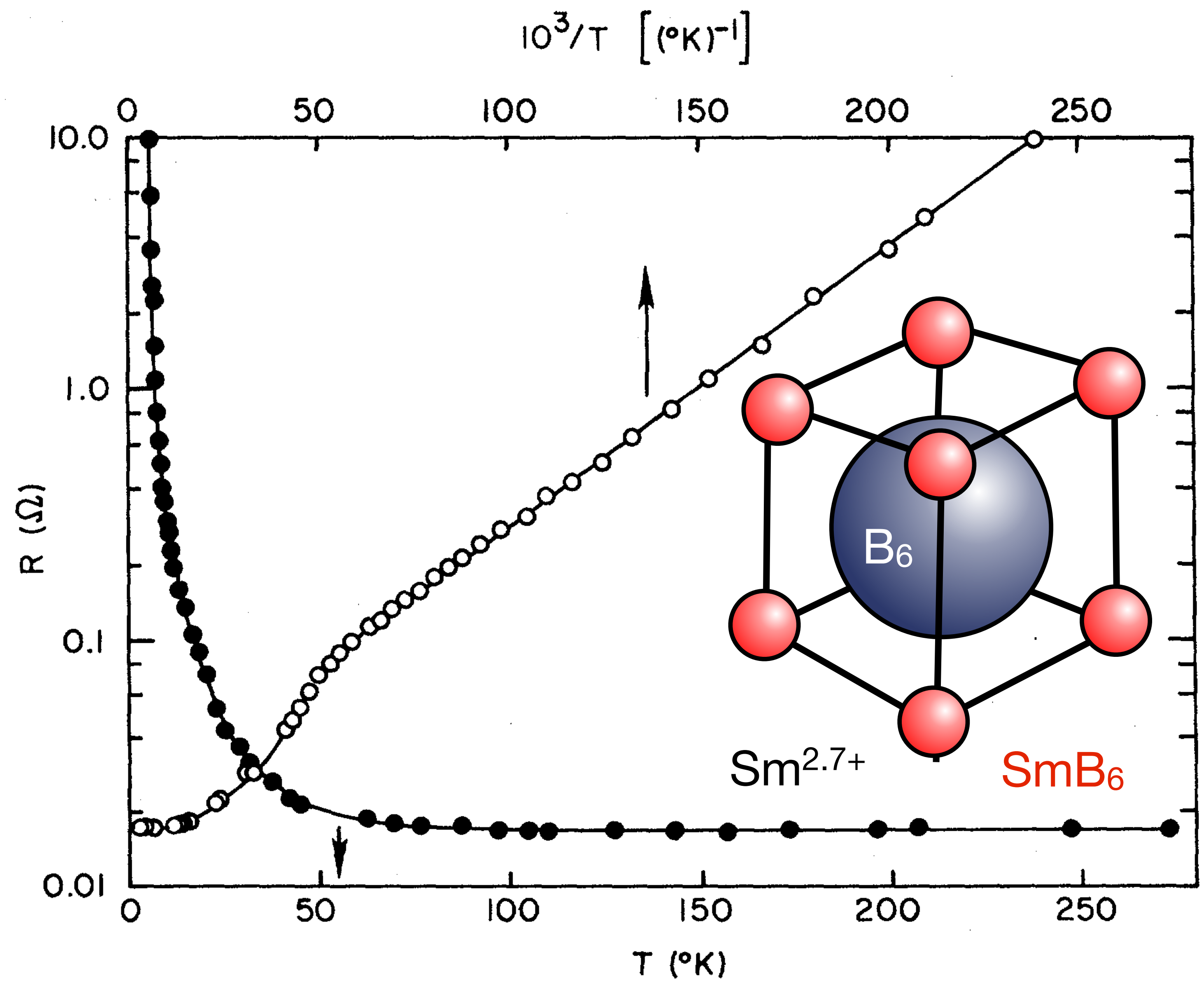


FIG. 1. Resistance of SmB_6 as a function of temperature. Closed circles: resistance versus T; open circles: resistance versus $10^3/T$.

Kondo insulators: History

Menth, Buehler and Geballe (PRL 22,295, 1969)
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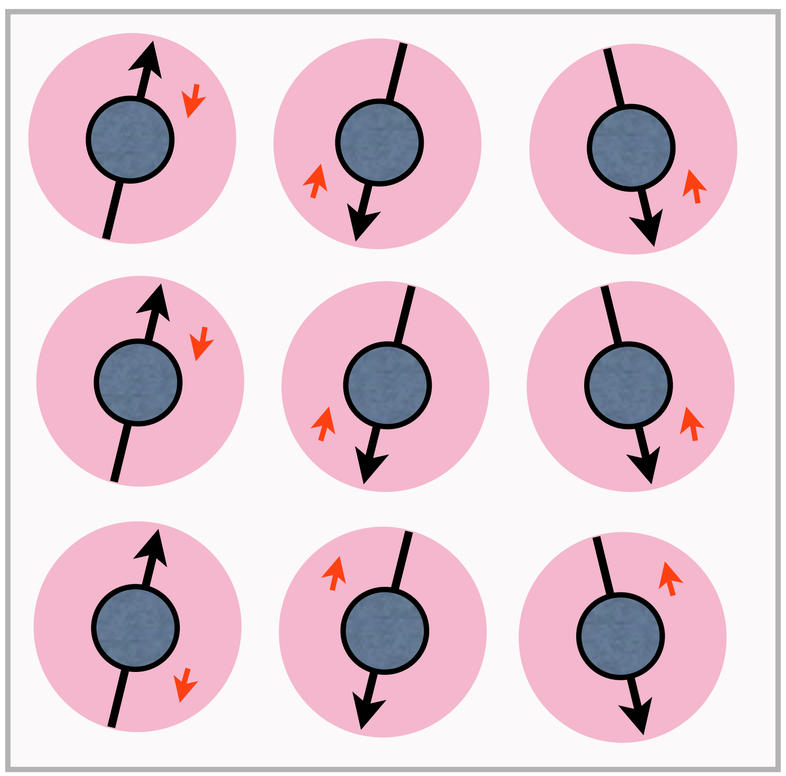
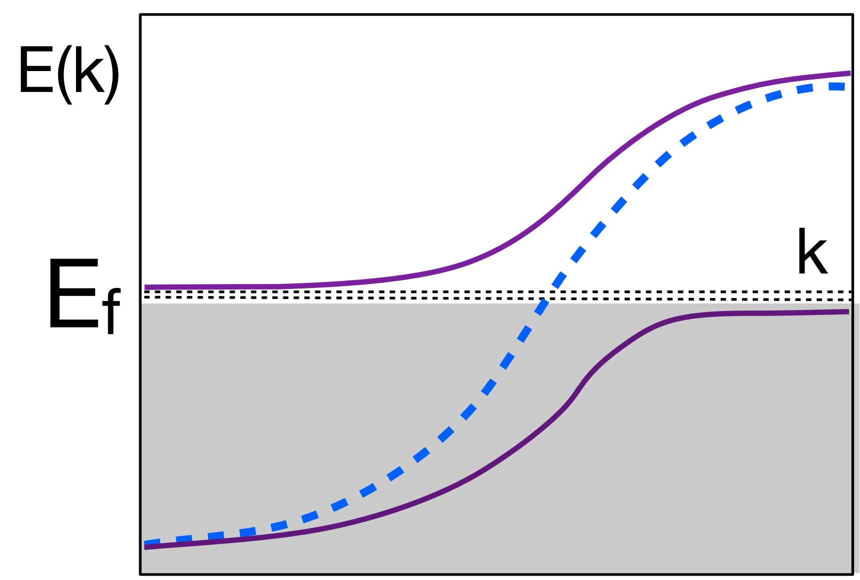
Simplest Kondo Lattice



Hybridization picture.

Maple + Wohlleben, 1972
Mott Phil Mag, 30,403,1974
Allen and Martin, 1979

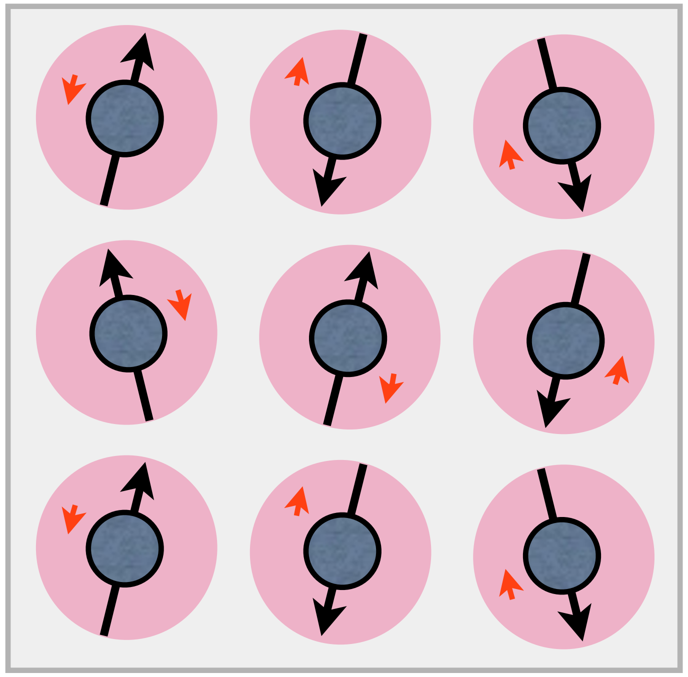
$$\mathcal{H} = (|\mathbf{k}\sigma\rangle V_{\sigma\alpha}(\mathbf{k})\langle\alpha| + \mathrm{H.c})$$



"In SmB6 and high-pressure SmS a very small gap separates occupied from unoccupied states, this in our view being due to hybridization of 4f and 4d bands." Mott 1974

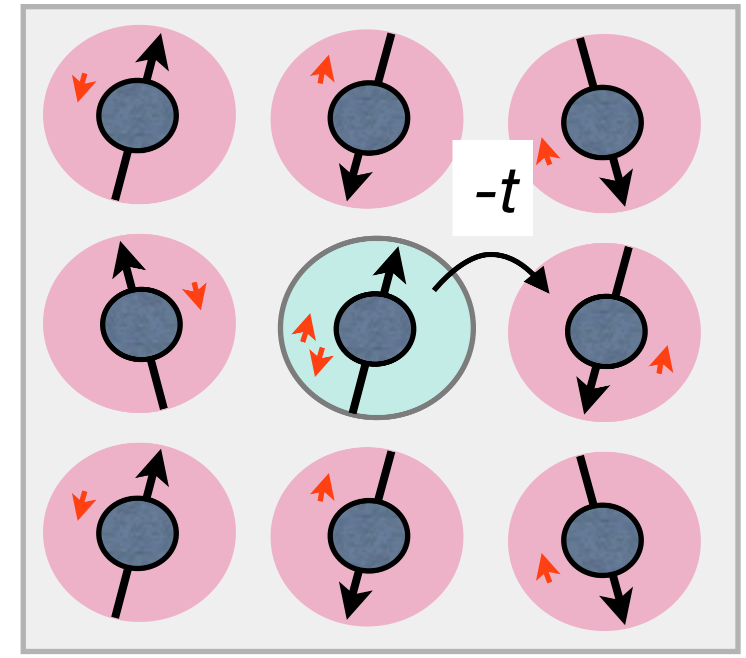
Strong coupling Kondo Lattice $J >> t$

$$H = J\sum \vec{\sigma}(j)\cdot\vec{S}_j - t\sum_{(i,j)}(c^{\dagger}_{i\sigma}c_{j\sigma} + \mathrm{H.c})$$



$n_e = n_{\rm spins}$

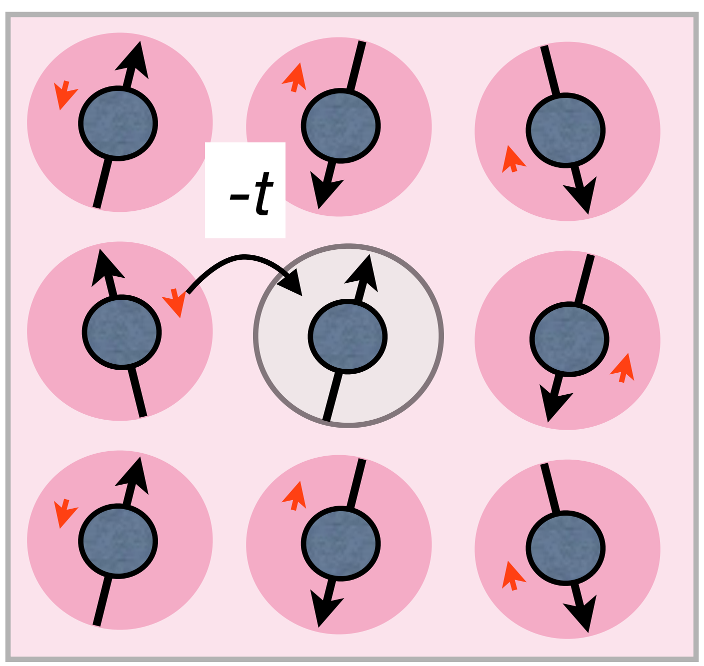
Kondo insulator



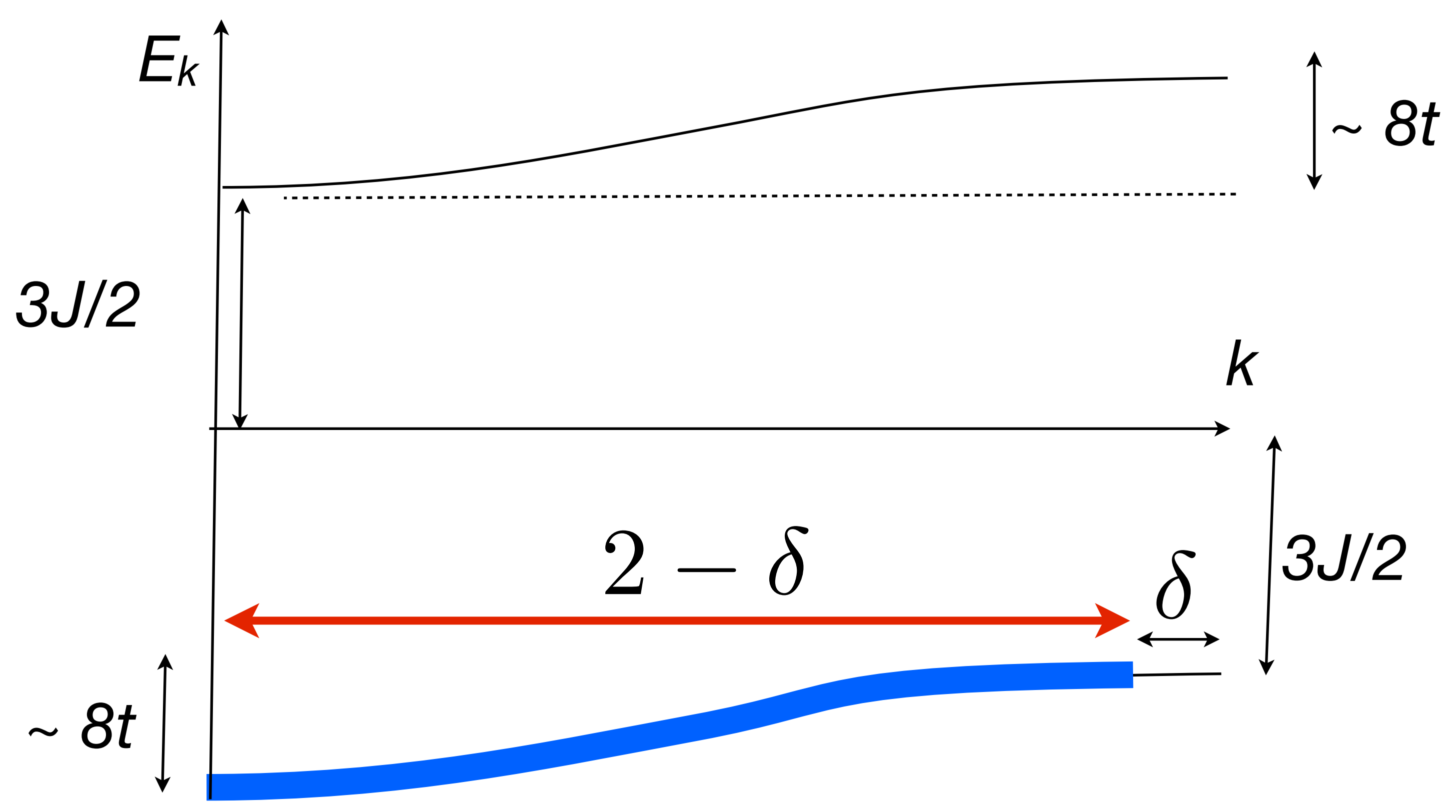
Electron doping
Mobile
“Heavy Electrons”

$$2\left(\frac{v_{\rm FS}}{(2\pi)^D}\right) = 2-\delta = n_{\rm spins} + n_e$$

FS sum rule counts spins as charged qp.



Hole doping: mobile heavy holes $n_e = n_{\rm spins} - \delta$

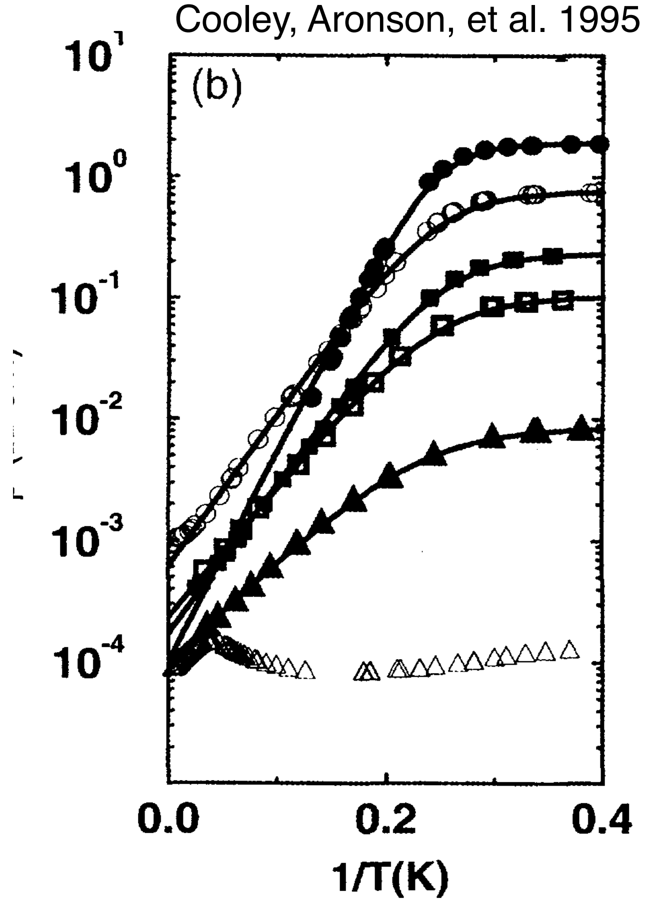


Kondo insulators: History

Menth, Buehler and Geballe (PRL 22,295, 1969)
Aeppli and Fisk (Comments CMP 16, 155, 1992)

Persistent conductivity Plateau

Cooley, Aronson, et al. 1995



Hybridization picture.

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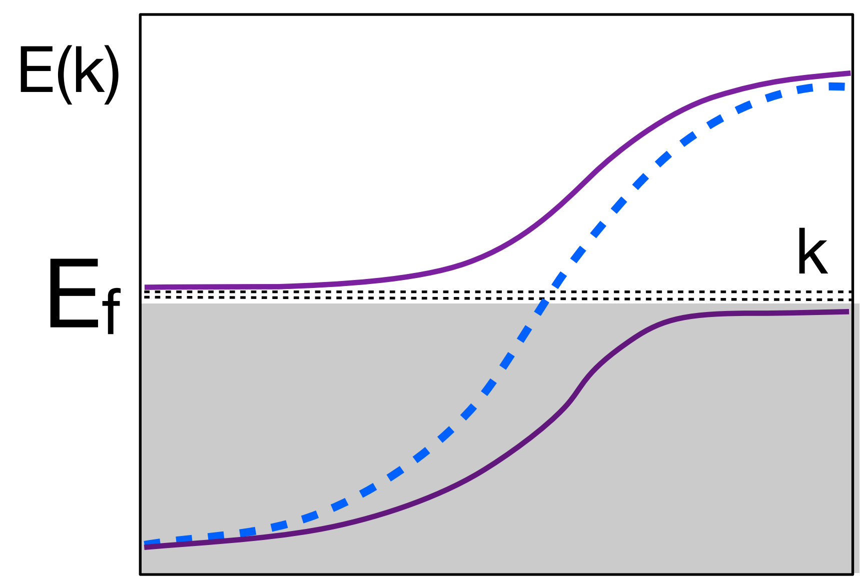


In SmB6 and high-pressure SmS a very small gap separates occupied from unoccupied states, this in our view being due to hybridization of 4f and 4d bands.

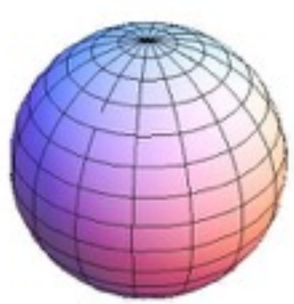
The rise of Topology.

"Gauss-Bonnet Theorem" Gauss (unpublished), Bonnet (1848)

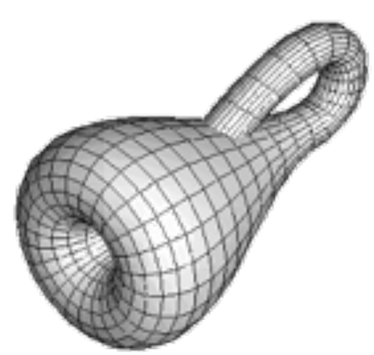
Differential Geometry $\longleftrightarrow$ Topology

$$\frac{1}{4\pi}\int \kappa dA = \frac{\Omega}{4\pi} = (1-g)$$

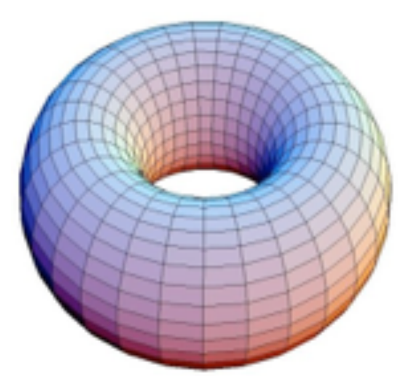
g=genus



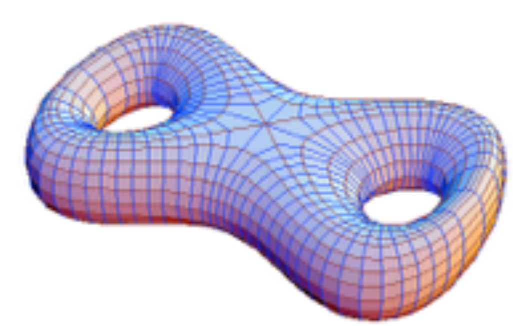
g=0



g=1



g=2



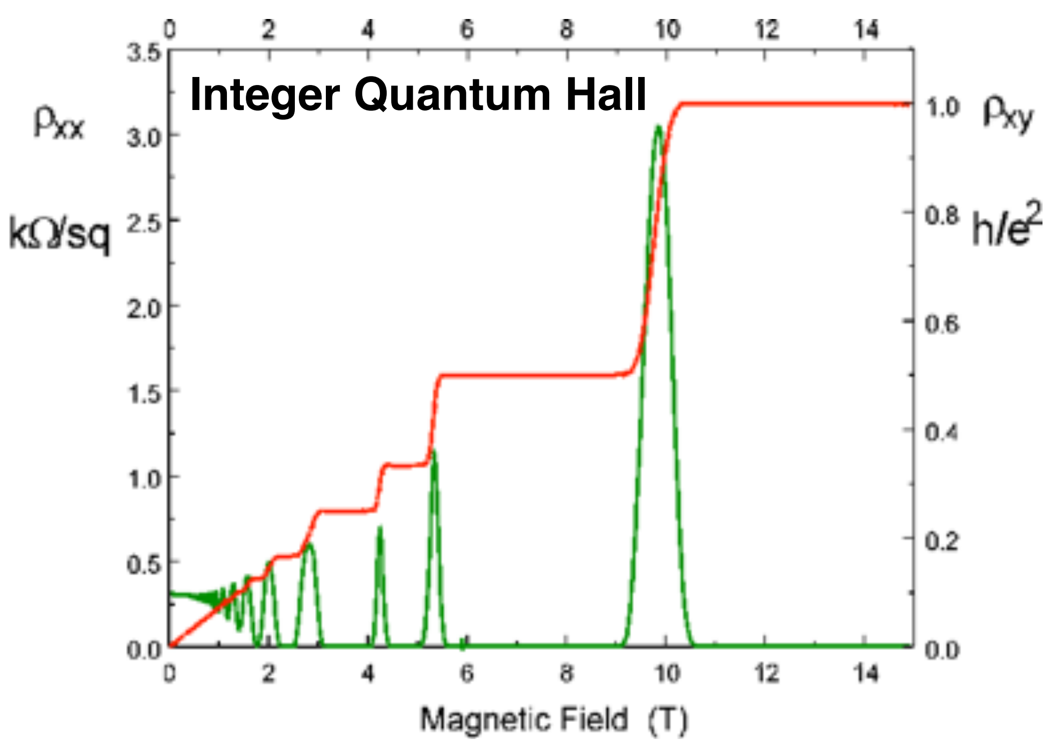
g=3

The rise of Topology.

Berry v. Klitzing Laughlin Thouless Haldane

Kane Mele Zhang Molencamp Hasan Balents Moore Roy Fu

Differential Geometry of the wavefunction ⟷ *Topological* order

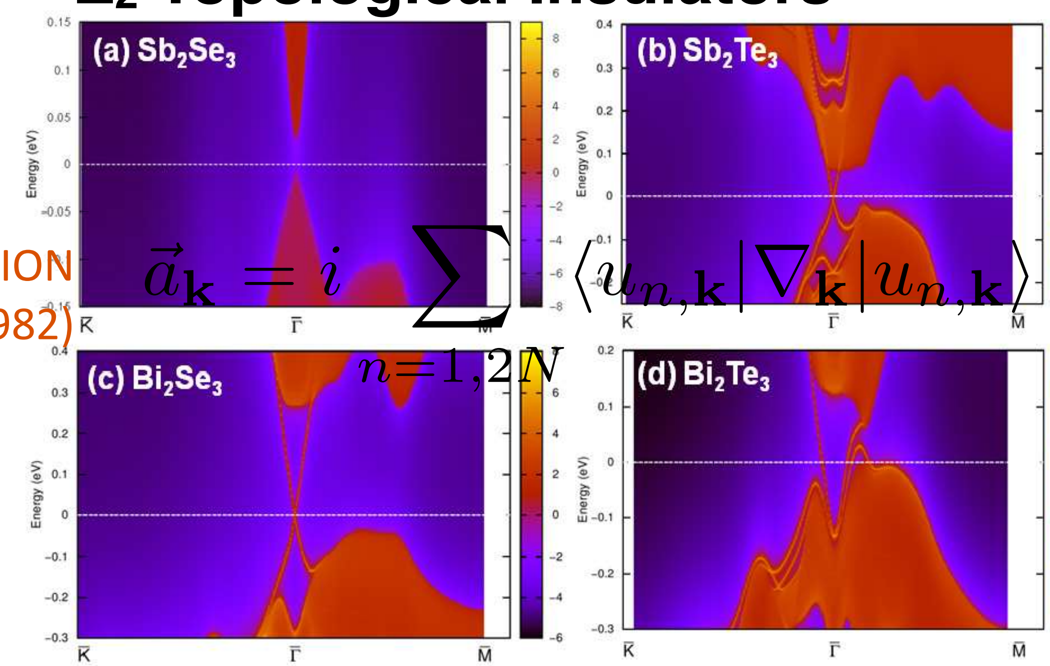


von Klitzing, Dorda & Pepper (1980)

BERRY CONNECTION
Thouless et al, (1982)

$$\vec{a}_{\mathbf{k}} = i \sum_{n=1,2N} \langle u_{n,\mathbf{k}} | \nabla_{\mathbf{k}} | u_{n,\mathbf{k}} \rangle$$

Z_2 Topological Insulators



Qi and Zhang, Rev. Mod Phys (2010).

1D Topological Insulator

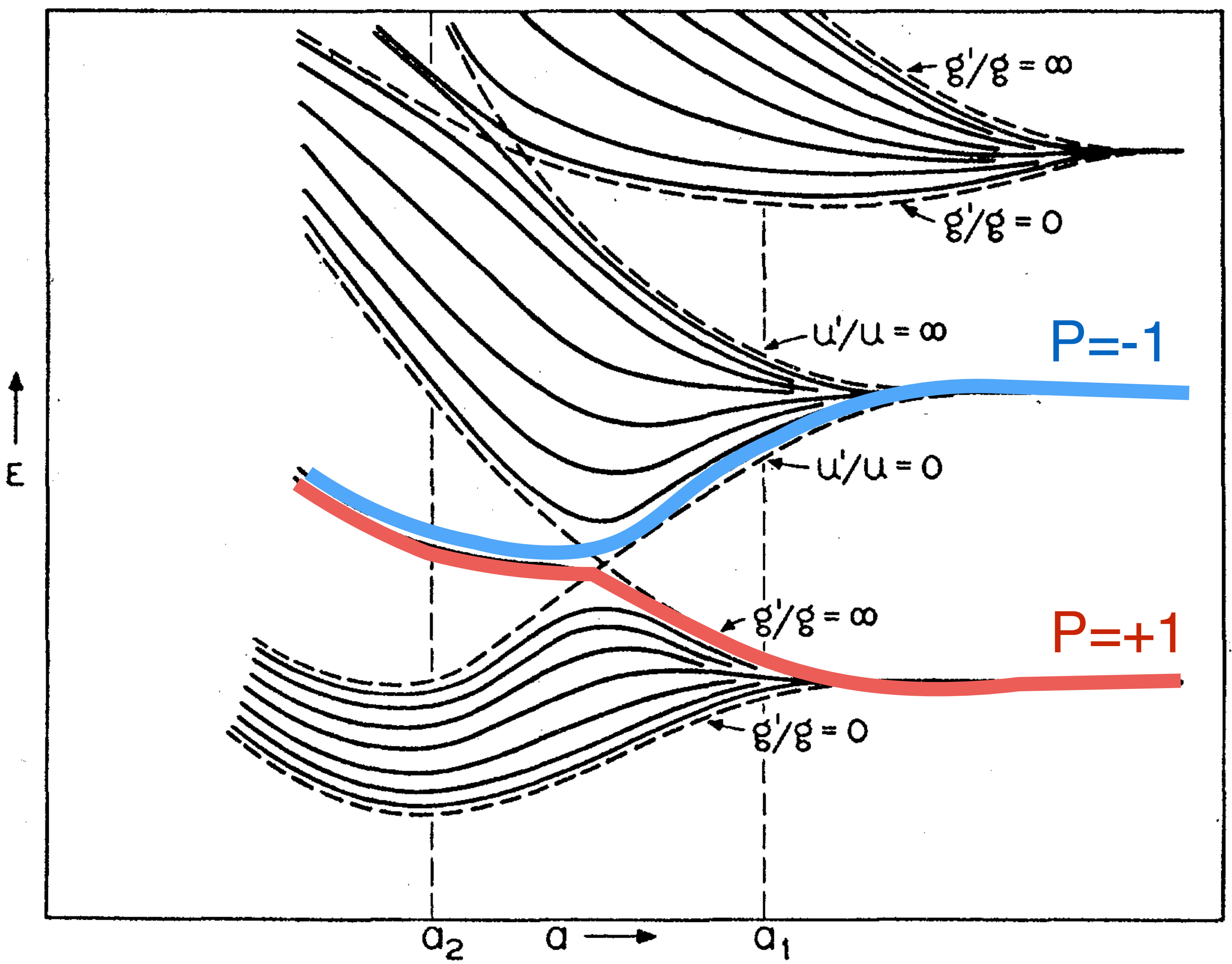
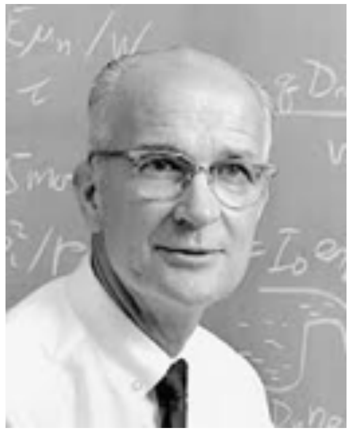
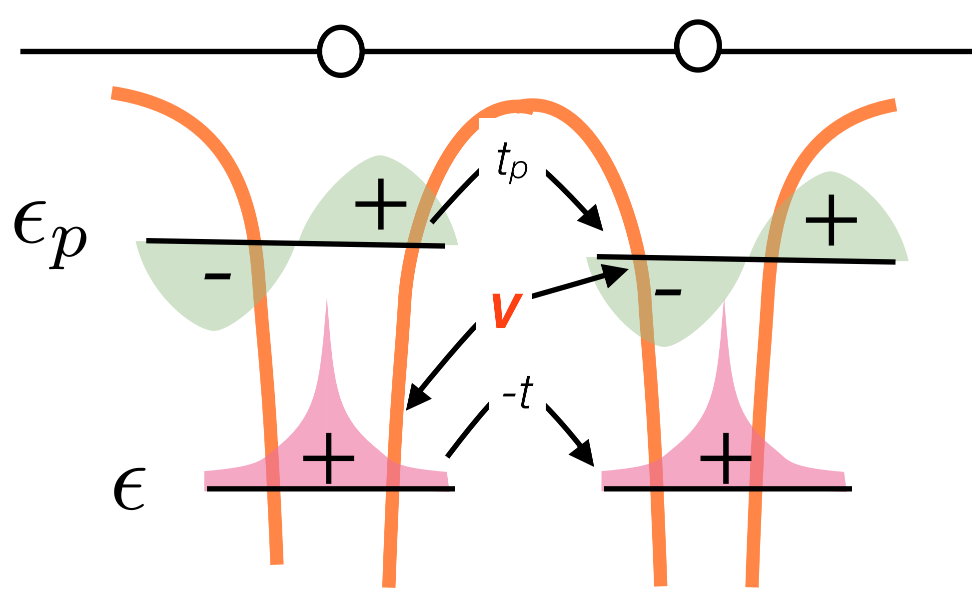


FIG. 2. Energy spectrum for a one-dimensional lattice with eight atoms.

Igor Tamm



William Shockley



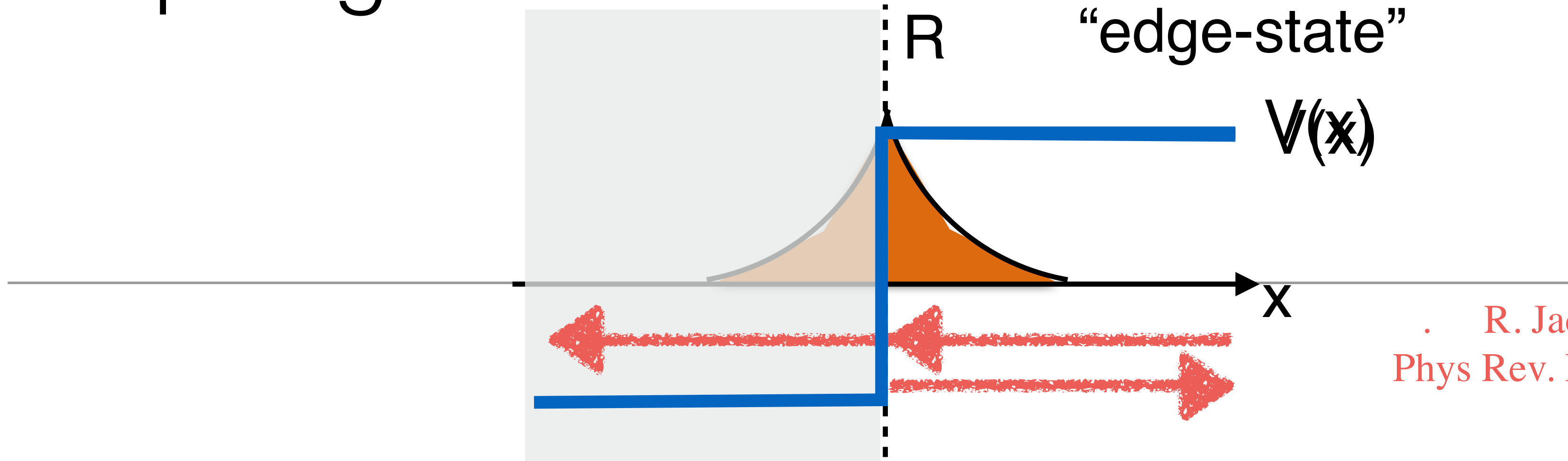
Tamm 1932, Shockley, Phys Rev, 56, 317 (1939): 1D TI

Open BCs- broken translation symmetry odd/even states mix to form edge states.

1D Topological Insulator

$V(x)=-V(-x)$ Odd Parity

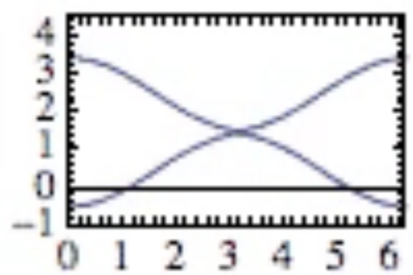
"edge-state"

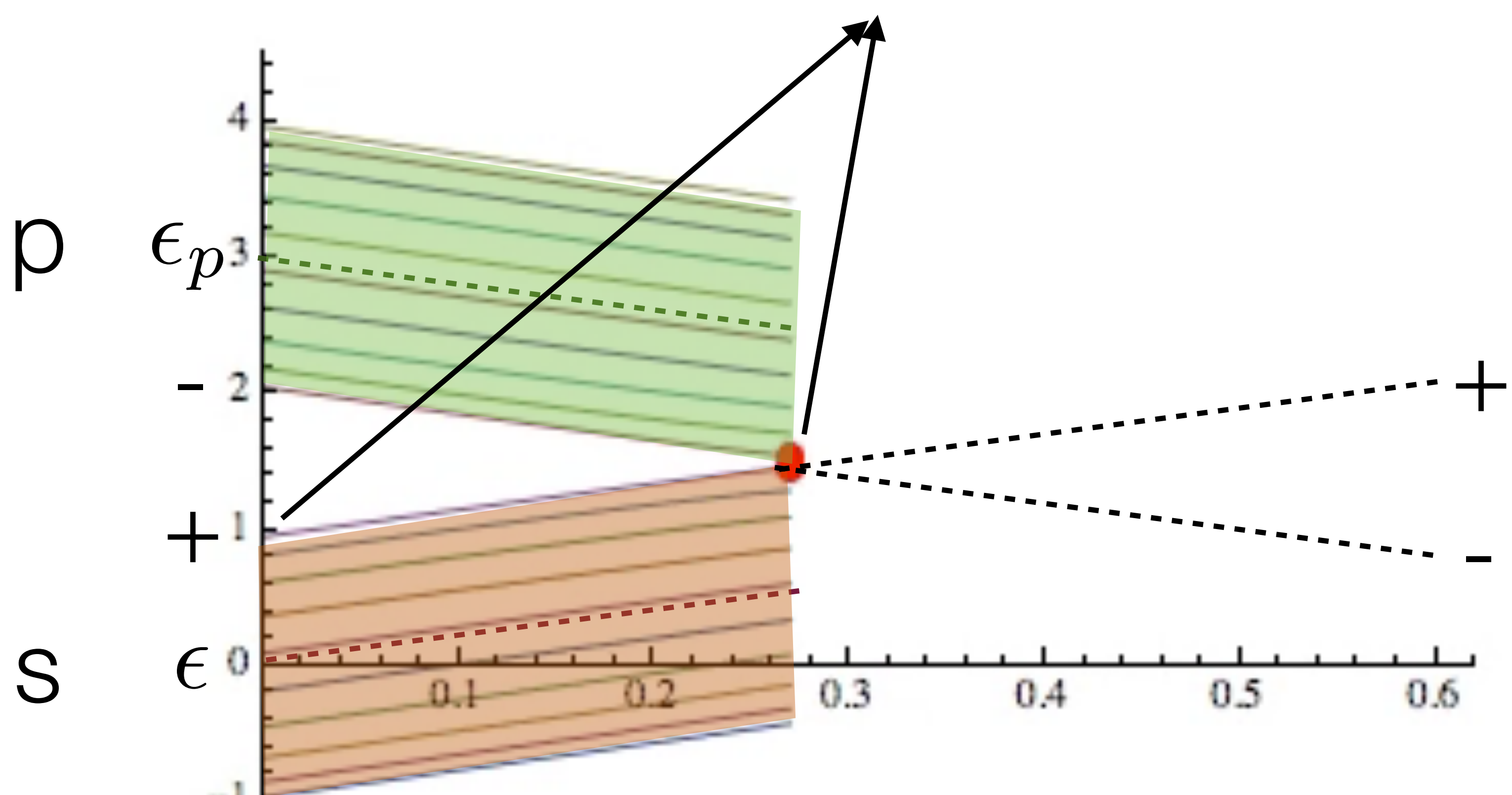


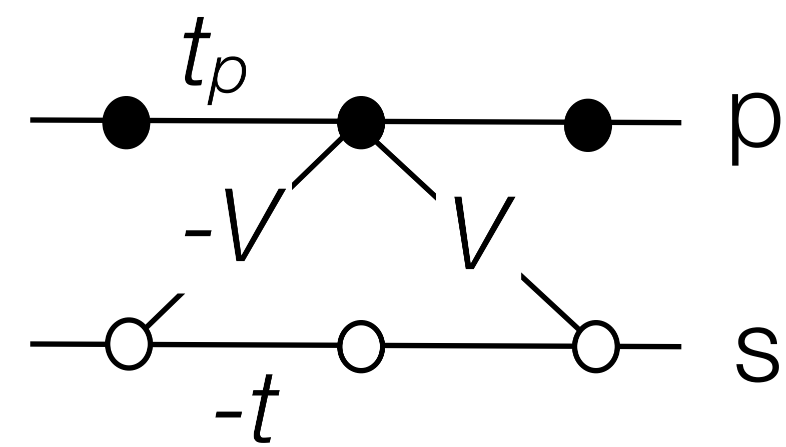
$$\begin{pmatrix} \epsilon & -t & 0 & 0 & 0 & 0 & 0 & V & 0 & 0 & 0 & 0 \\ -t & \epsilon & -t & 0 & 0 & 0 & -V & 0 & V & 0 & 0 & 0 \\ 0 & -t & \epsilon & -t & 0 & 0 & 0 & -V & 0 & V & 0 & 0 \\ 0 & 0 & -t & \epsilon & -t & 0 & 0 & 0 & -V & 0 & V & 0 \\ 0 & 0 & 0 & -t & \epsilon & -t & 0 & 0 & 0 & -V & 0 & V \\ 0 & 0 & 0 & 0 & -t & \epsilon & 0 & 0 & 0 & 0 & -V & 0 \\ 0 & -V & 0 & 0 & 0 & 0 & \epsilon p & tp & 0 & 0 & 0 & 0 \\ V & 0 & -V & 0 & 0 & 0 & tp & \epsilon p & tp & 0 & 0 & 0 \\ 0 & V & 0 & -V & 0 & 0 & 0 & tp & \epsilon p & tp & 0 & 0 \\ 0 & 0 & V & 0 & -V & 0 & 0 & 0 & tp & \epsilon p & tp & 0 \\ 0 & 0 & 0 & V & 0 & -V & 0 & 0 & 0 & tp & \epsilon p & tp \\ 0 & 0 & 0 & 0 & V & 0 & 0 & 0 & 0 & 0 & tp & \epsilon p \end{pmatrix}$$

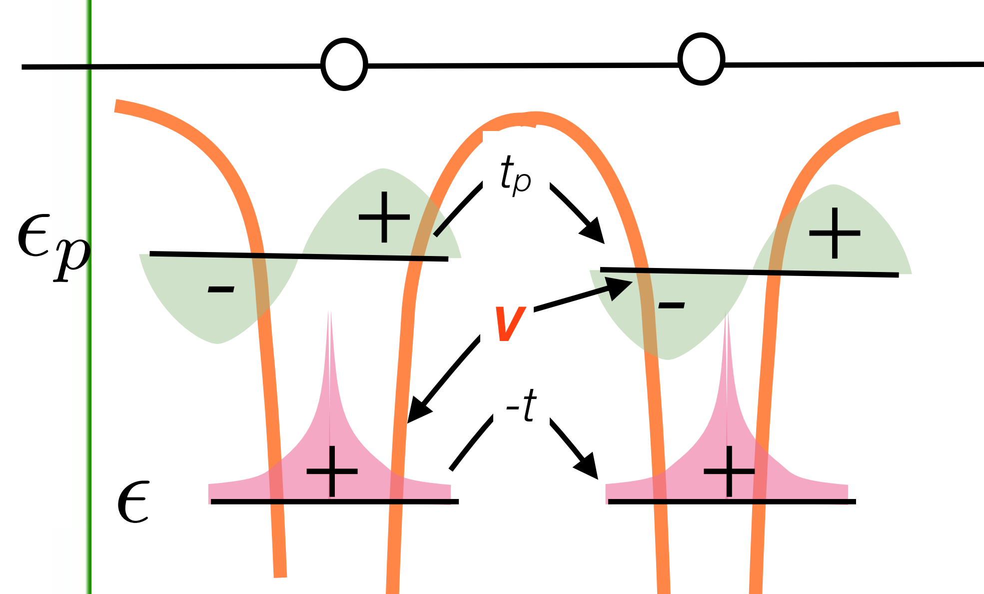
R. Jackiw and C. Rebbi,
Phys Rev. D13, 3398 (1976)

Band Structure





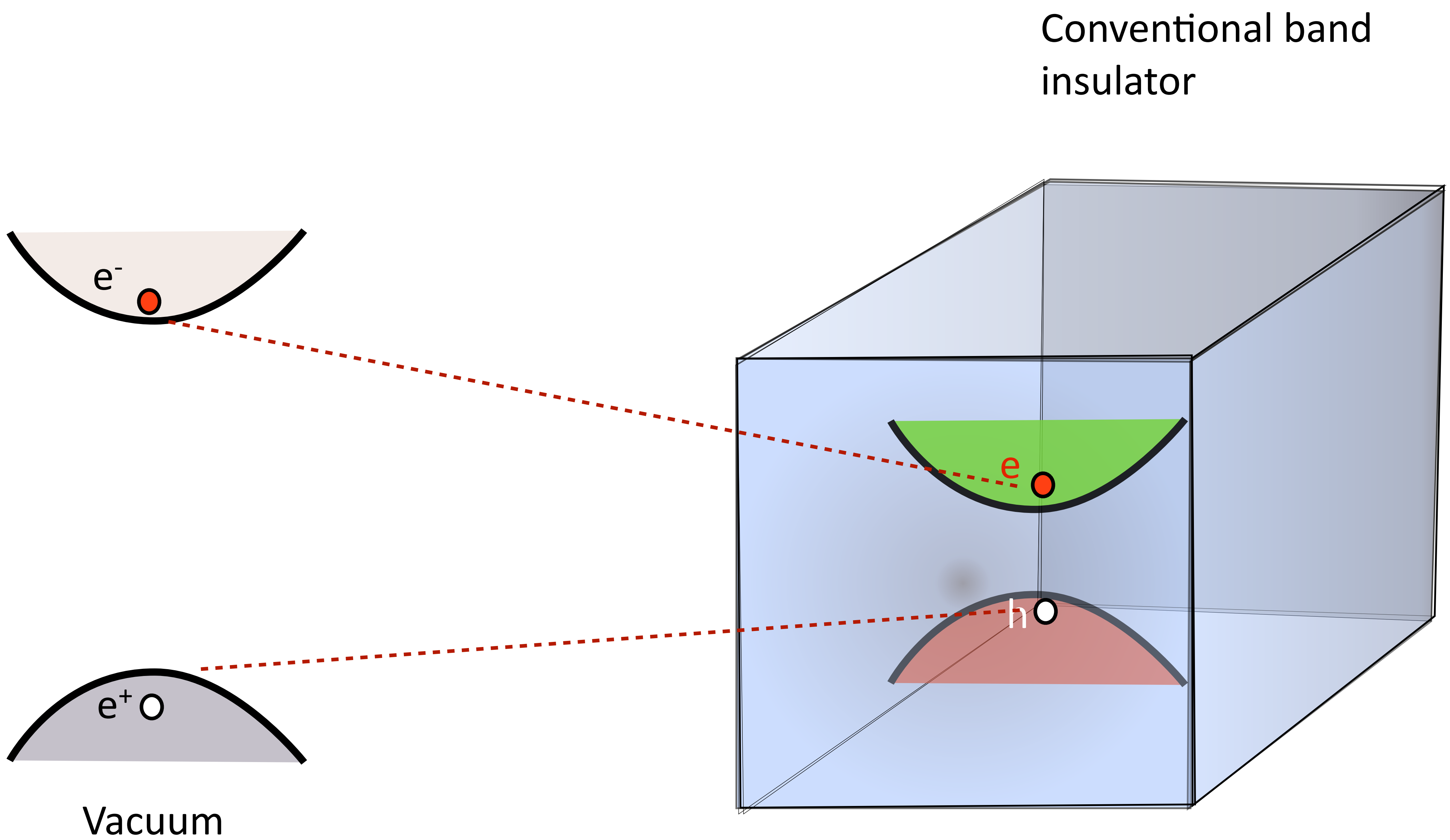




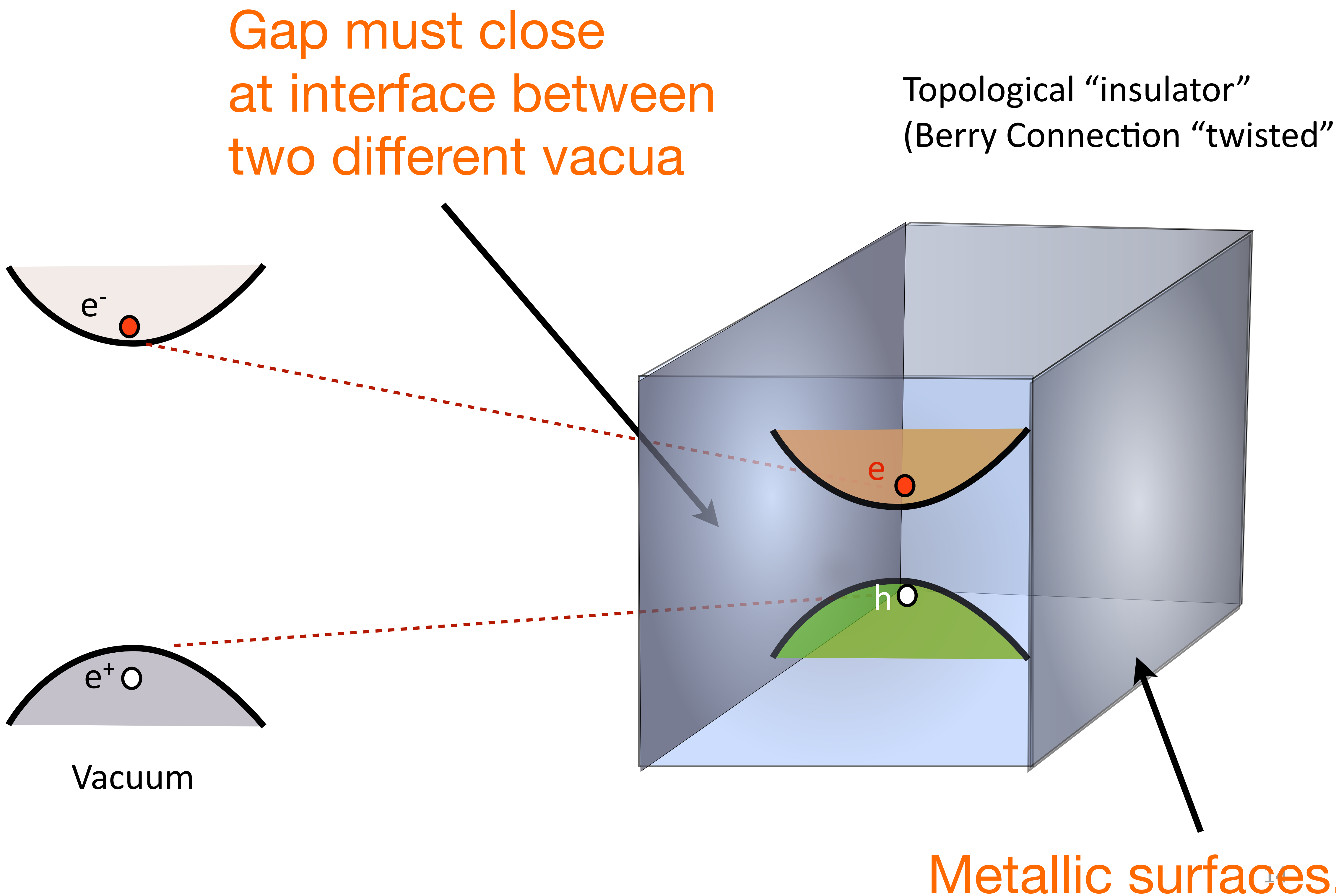
With periodic BCs- parity conserved-odd and even states **cross**.

With open BCs- parity broken -Odd/ even states mix - avoided crossing, so form edge states.

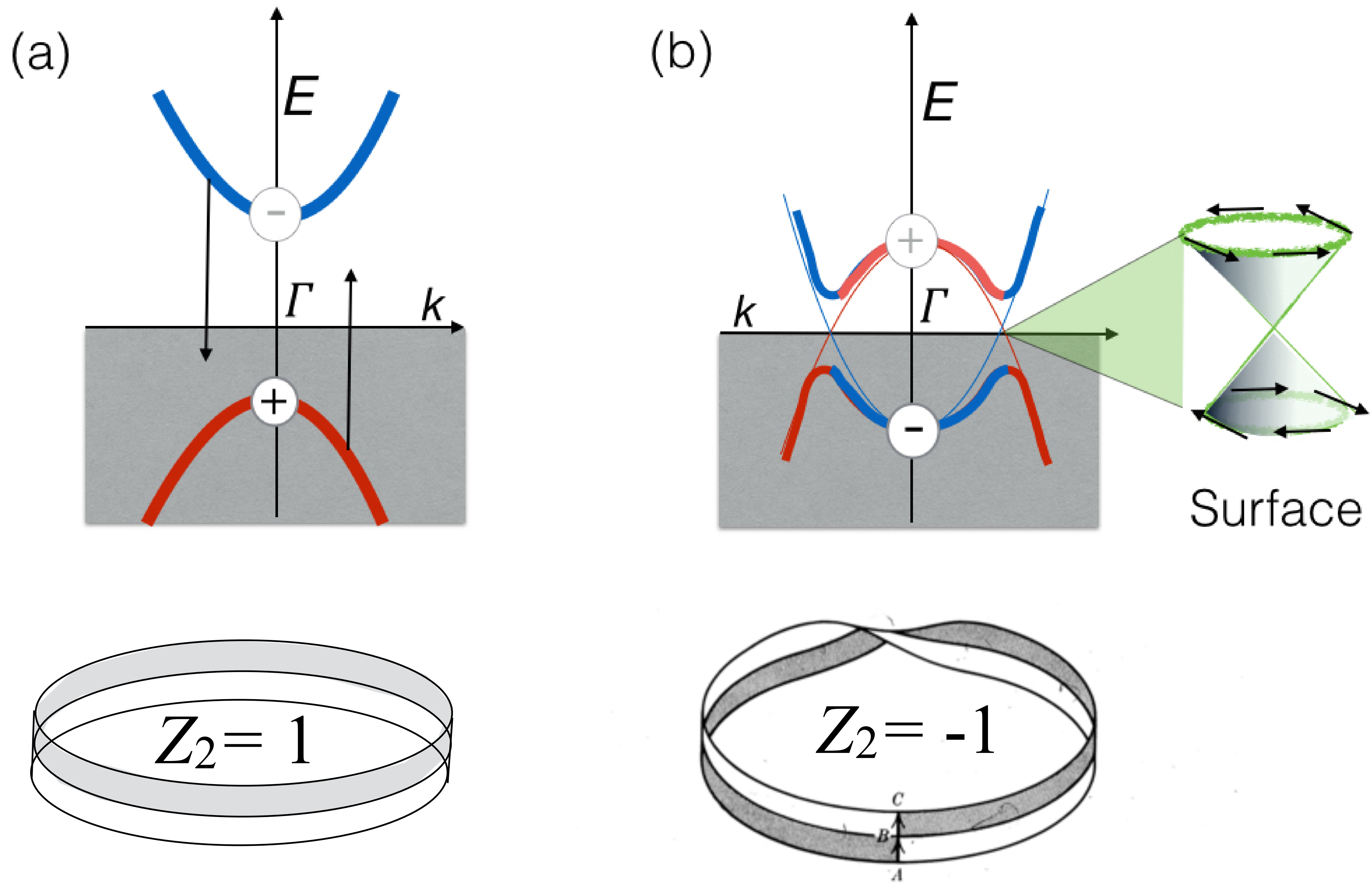
Conventional band insulator:
adiabatic continuation of the vacuum.



Topological insulator : adiabatically disconnected from the vacuum.



Band Crossing of odd and even parity states Yields a Z_2 Topological Insulator (Fu, Kane, Mele, 2007)

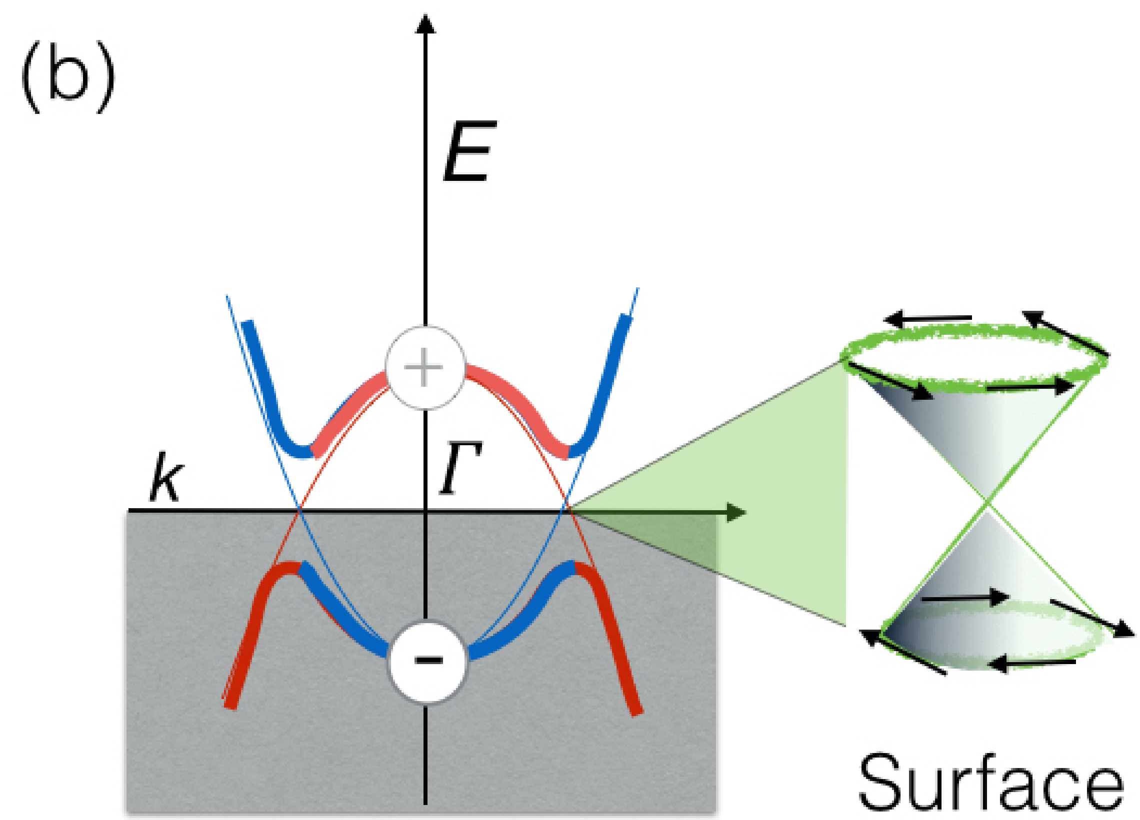


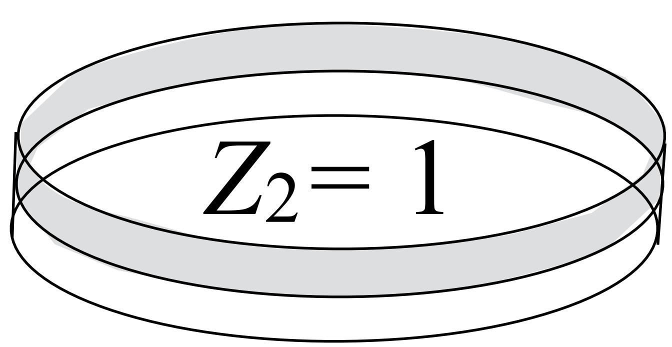
Topological Texture of Berry Connection

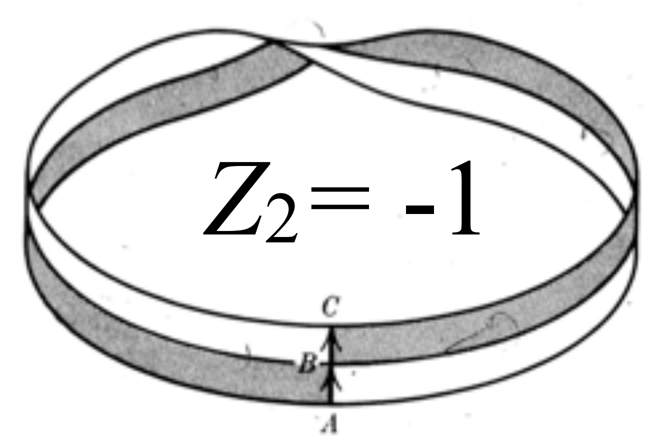
Band Crossing of odd and even parity states Yields a Z_2 Topological Insulator (Fu, Kane, Mele, 2007)

$$Z_2 = \prod_i \delta(\Gamma_i)$$

Fu and Kane (2008) :Parity equation.







Topological Texture of Berry Connection

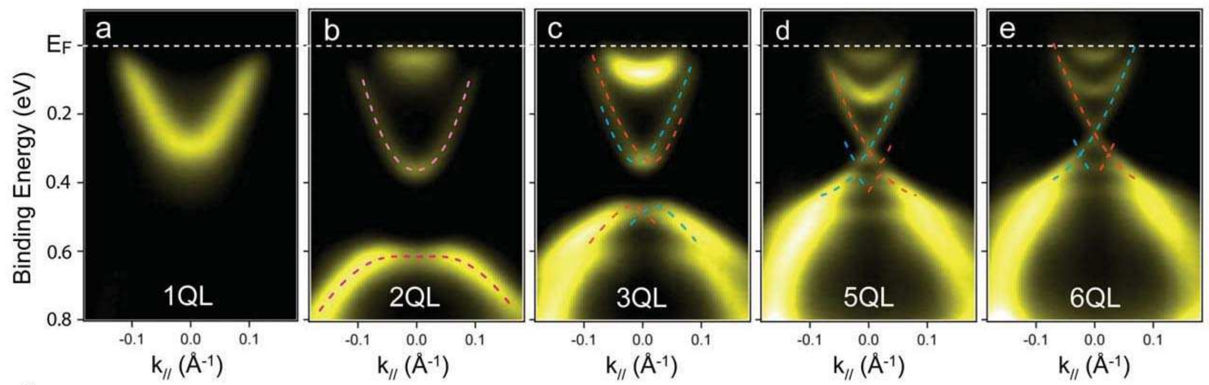


FIG. 27 ARPES data for Bi_2Se_3 thin films of thickness (a) 1QL (b) 2QL (c) 3QL (d) 5QL (e) 6QL, measured at room temperature (QL stands for quintuple layer). From Zhang *et al.*, 2009.

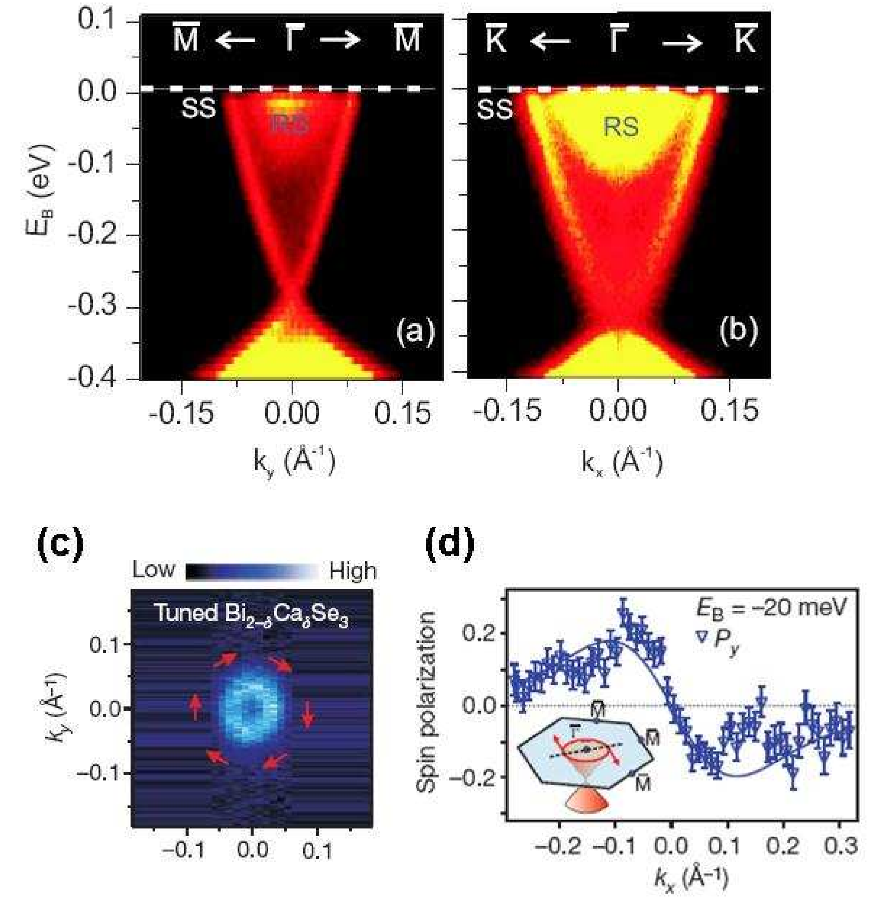


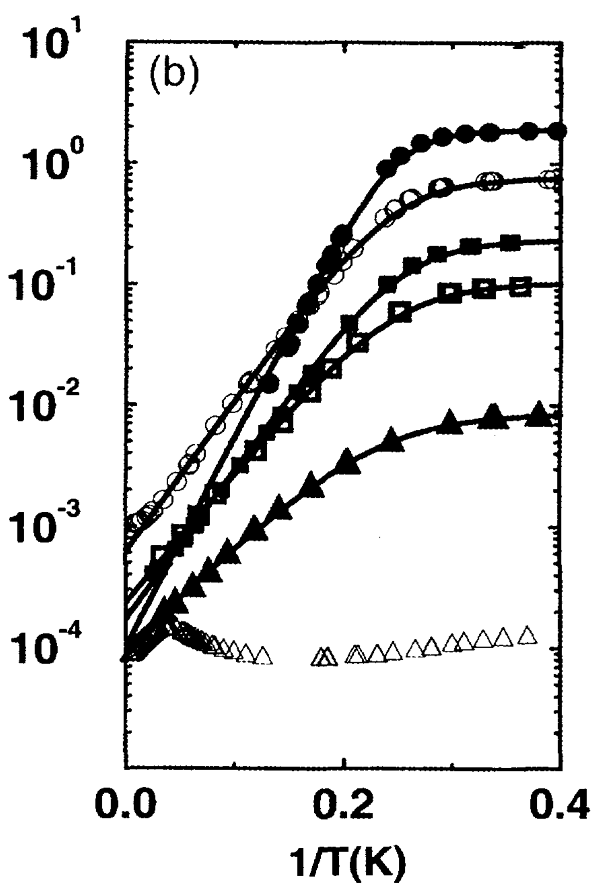
FIG. 25 ARPES data for the dispersion of the surface states of Bi_2Se_3, along directions (a) $\bar{\Gamma} - \bar{M}$ and (b) $\bar{\Gamma} - \bar{K}$ in the surface Brillioun zone. Spin-resolved ARPES data is shown along $\bar{\Gamma} - \bar{M}$ for a fixed energy in (d), from which the spin polarization in momentum space (c) can be extracted. From Xia *et al.*, 2009 and Hsieh *et al.*, 2009.

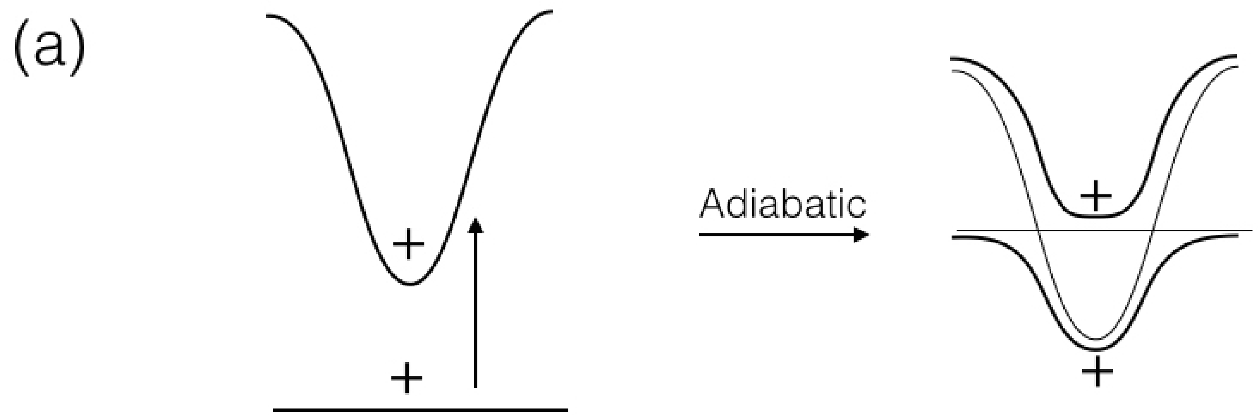
- 2D HgTe/ CdTe Quantum Wells (Konig et al, 07/8)
- 3D Bi_2Se_3 , Bi_2Te_3, Sb_2Te_3 (Zhang et al ,Xia et al ,Chen et al, Hsieh et al (09))

Are there strongly correlated counterparts?
f electrons?
Strongly interacting, infinite Spin orbit, odd parity.

Persistent conductivity Plateau

Are Kondo insulators topological?





R. Martin & J. Allen, J. Applied Physics, **50,**7561 (1979)

Dzero, Sun, Galitski, PC Phys. Rev. Lett. **104**, 106408 (2010)

Many Body Localized

Many Body Delocalization

Band Theory SmB_6: T. Takimoto, J. Phys. Soc. Jpn. 80, 123710 (2011).

Maxim Dzero, Kai Sun, Piers Coleman and Victor Galitski, Phys. Rev. B 85 , 045130-045140 (2012).

Gutzwiller + Band Theory F. Lu, J. Zhao, H. Weng, Z. Fang and X. Dai, Phys. Rev. Lett. 110, 096401 (2013).

Victor Alexandrov, Maxim Dzero and Piers Coleman PRL (2013).

dHvA LaB_6

(parent compound without f-electrons: $4f^0$)

VIEW B VOLUME 13, NUMBER 12

de Haas–van Alphen effect and the Fermi surface of LaB_6†

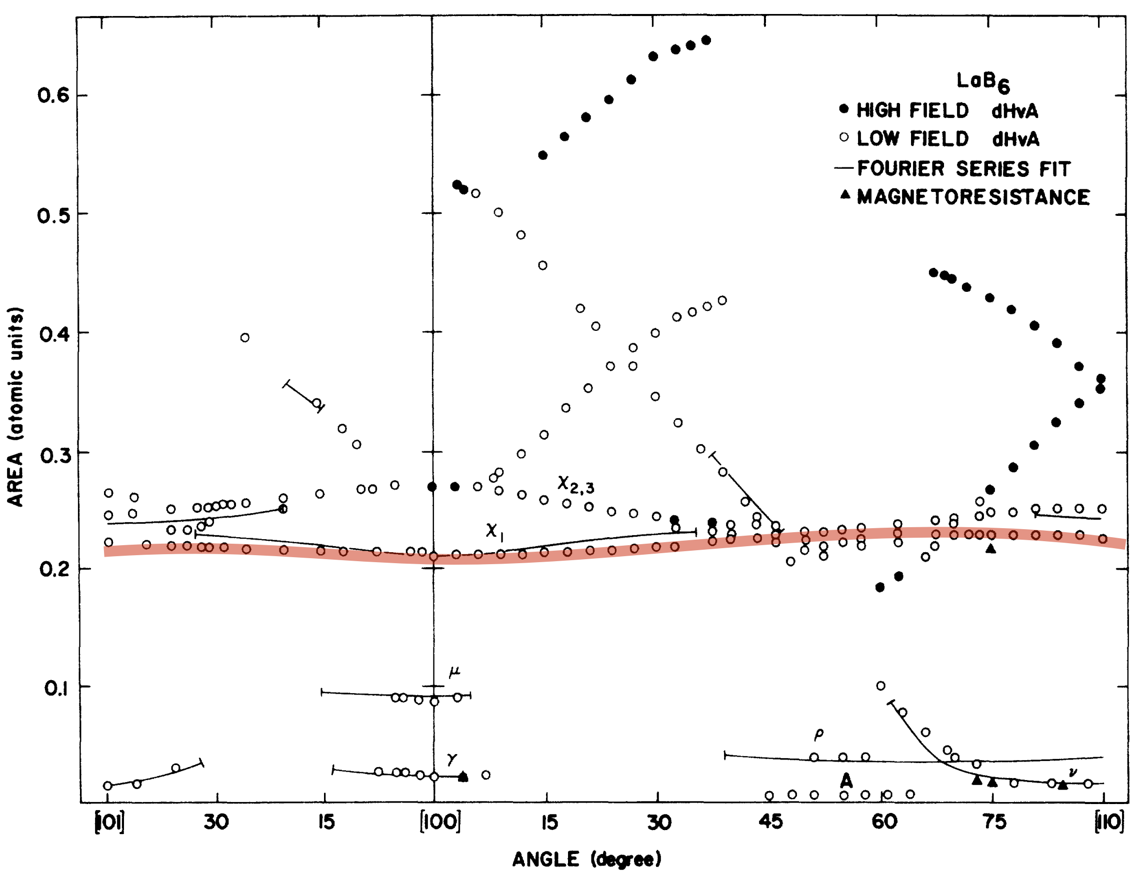
A. J. Arko, G. Crabtree, D. Karim, F. M. Mueller,* and L. R. Windmiller
Argonne National Laboratory, Argonne, Illinois 60439

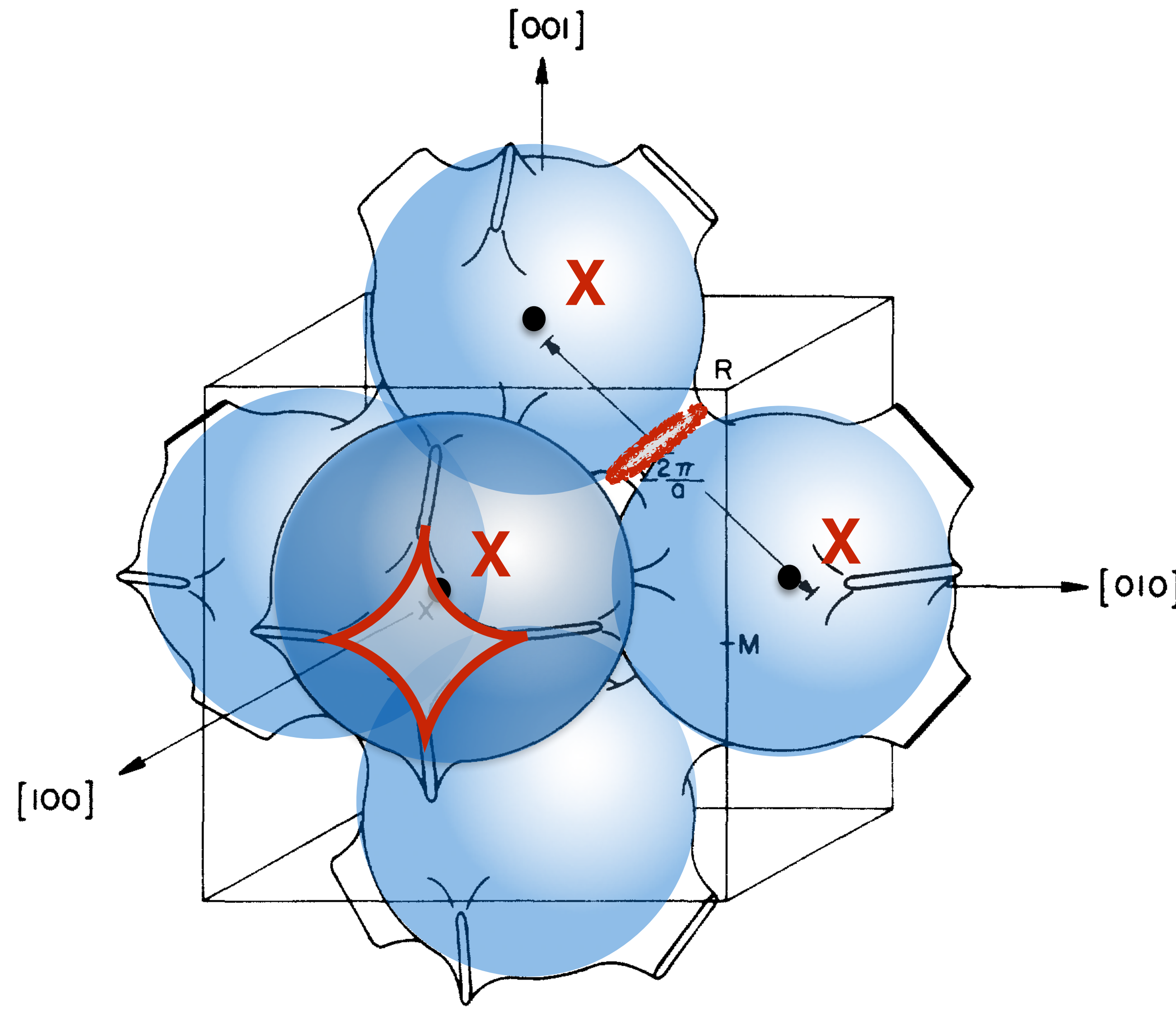
J. B. Ketterson
Department of Physics, Northwestern University, Evanston, Illinois 60201 and Argonne National Laboratory, Argonne, Illinois 60439

Z. Fisk
Department of Physics, University of California, San Diego, La Jolla, California 92037

(Received 19 February 1976)

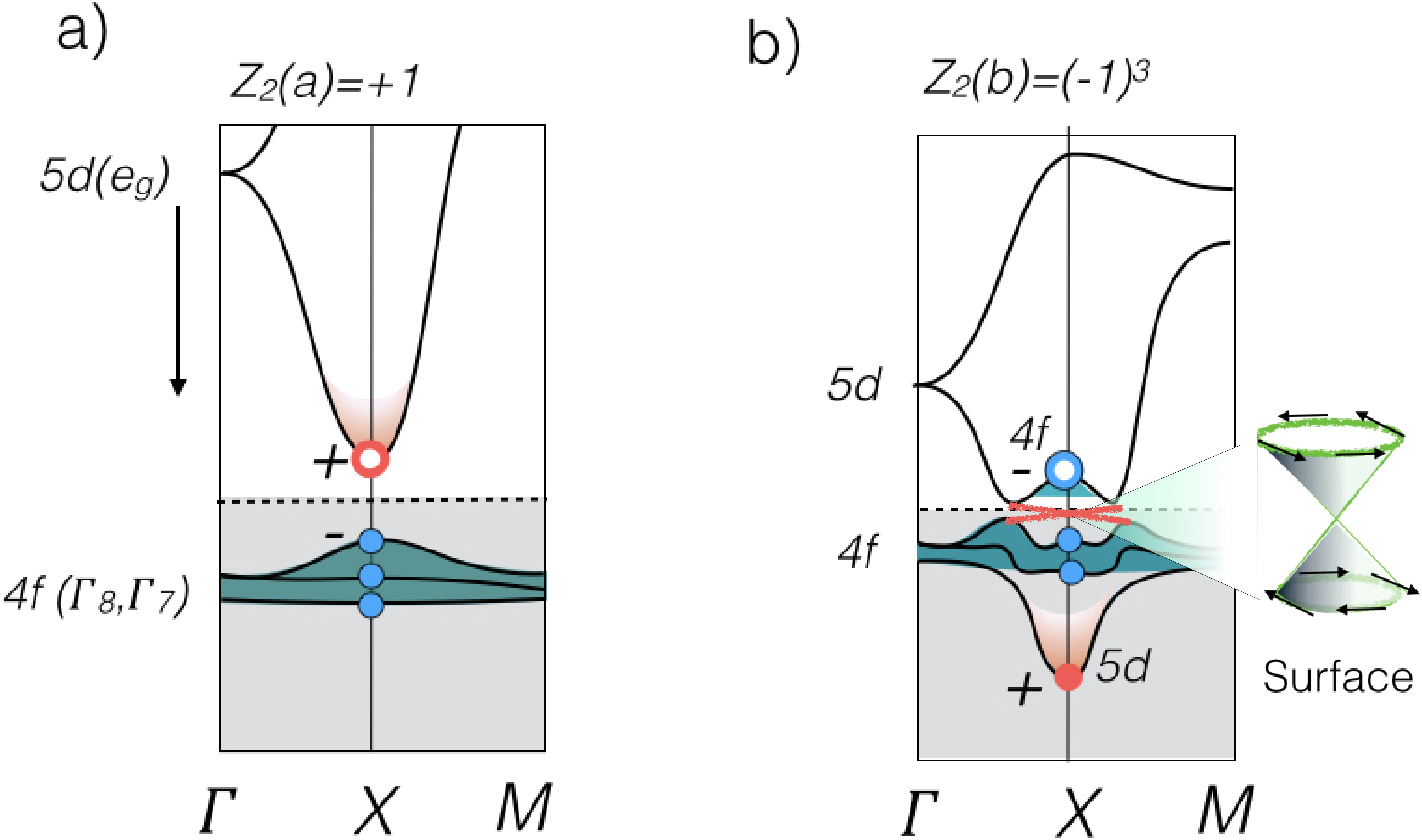
d-bands form around the X Points.





Features of the new model

Dzero et al, Annual Reviews of Condensed Matter Physics (2016), arXiv 1506.05635



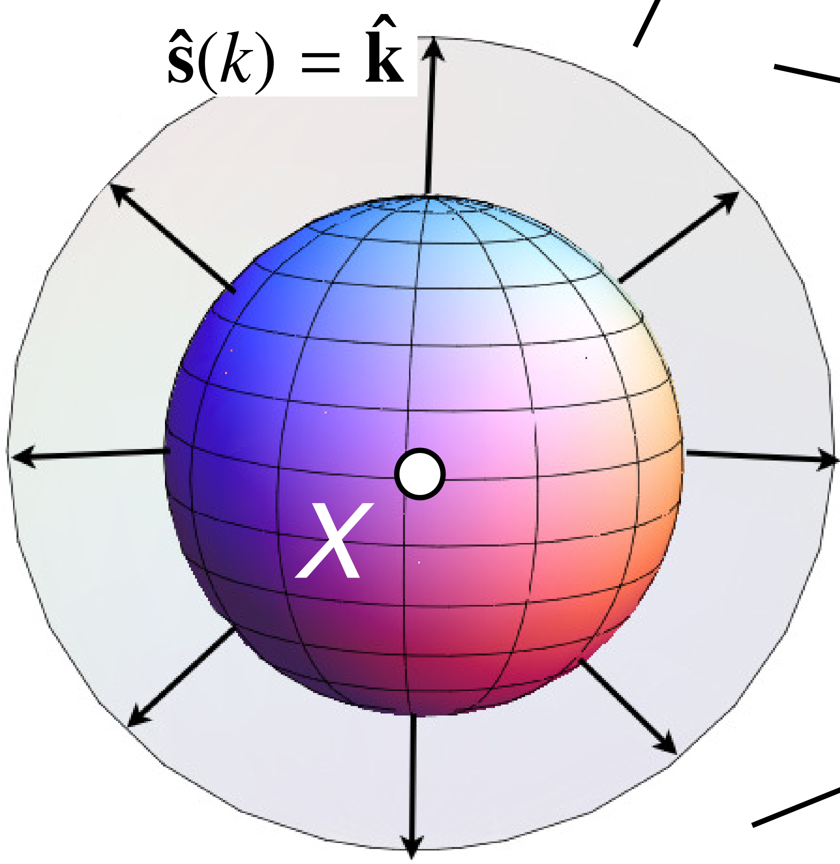
Three crossings: THREE DIRAC CONES ON SURFACE.

Features of the new model

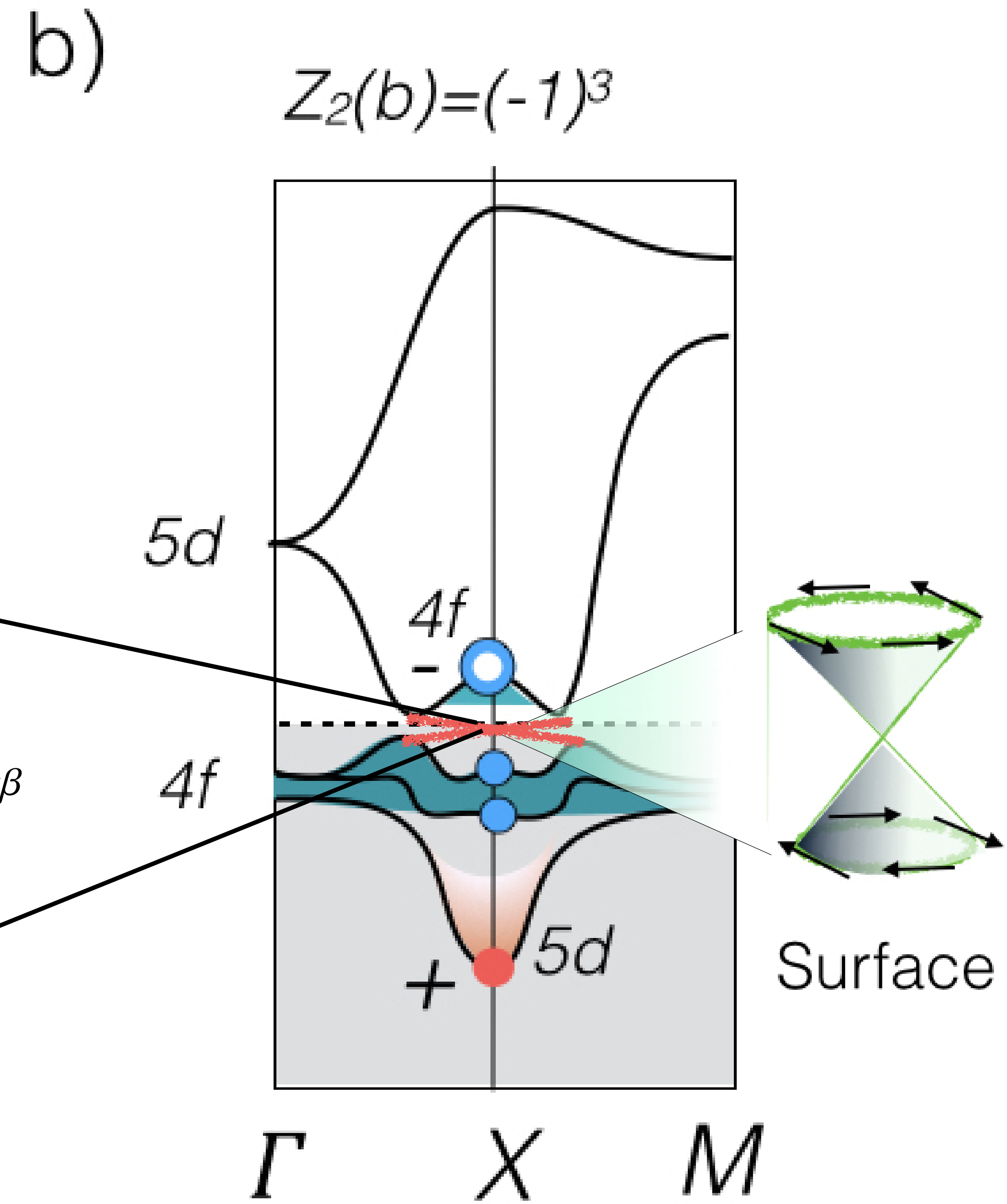
Dzero et al, Annual Reviews of Condensed Matter Physics (2016), arXiv 1506.05635

Like He-3B: an adaptive insulator.

$$\mathcal{H}(\mathbf{k}) = \left(\begin{array}{c|c} \epsilon_{\mathbf{k}} & V\,\mathbf{s}_{\mathbf{k}}\cdot\vec{\sigma} \\ \hline V\,\mathbf{s}_{\mathbf{k}}\cdot\vec{\sigma} & \epsilon_{f\mathbf{k}} \end{array}\right)$$



$$V_{\alpha\beta}(k) = V\mathbf{s}_{\mathbf{k}}\cdot\vec{\sigma}_{\alpha\beta}$$



$$\mathbf{s}_{\mathbf{k}} = (\sin k_x, \sin k_y, \sin k_z) \sim \hat{\mathbf{k}}$$

Three crossings: THREE DIRAC CONES ON SURFACE.

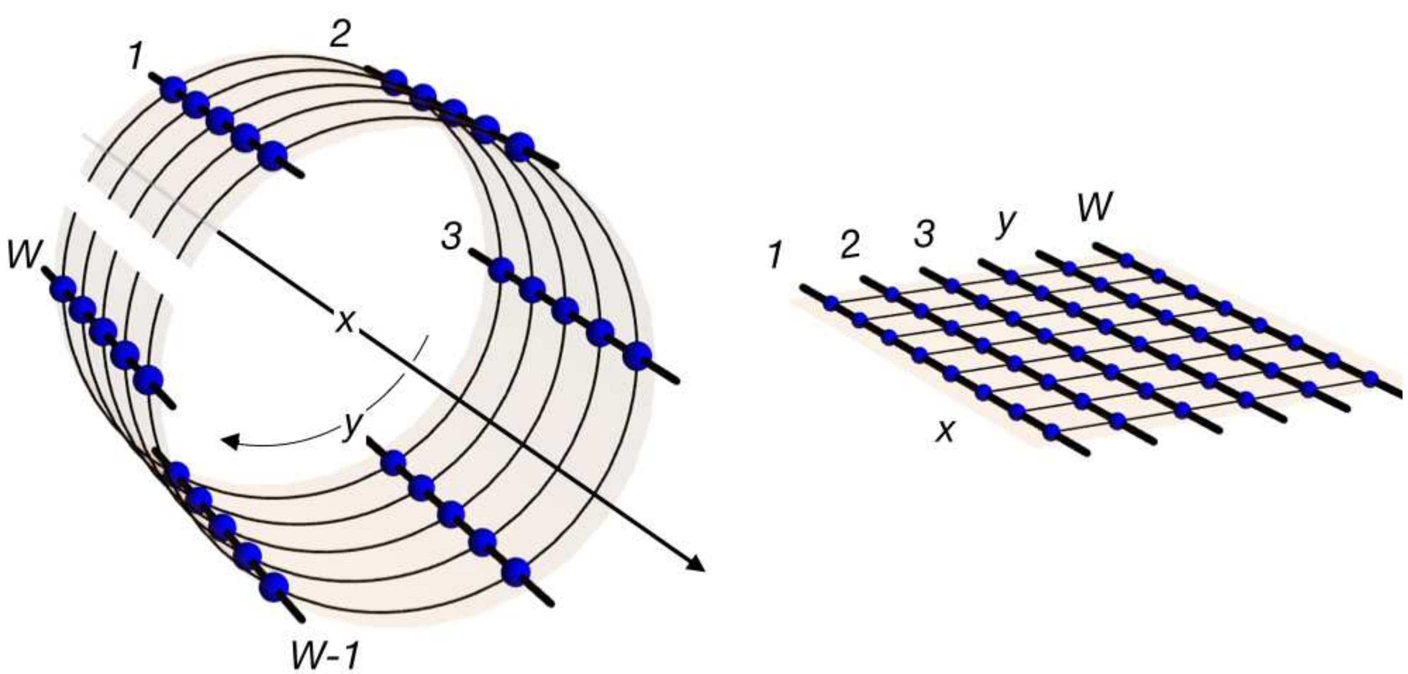
Hybridization of **f (P=+)** and **d** (P=-) vanishes at X point.

Strip Calculation.

$$H_{MF} = \sum_{\mathbf{k}} \left(\psi^{\dagger}{}_{\mathbf{k}\uparrow} \underline{h}(\mathbf{k}) \psi_{\mathbf{k}\uparrow} + \psi^{\dagger}{}_{\mathbf{k}\downarrow} \underline{h}^{*}(\mathbf{k}) \psi_{\mathbf{k}\downarrow} \right)$$

$$\underline{h}(\mathbf{k}) = \begin{pmatrix} \epsilon_{\mathbf{k}} & \tilde{V}(s_x - i s_y) \\ \tilde{V}(s_x + i s_y) & \epsilon_{f\mathbf{k}} \end{pmatrix}.$$

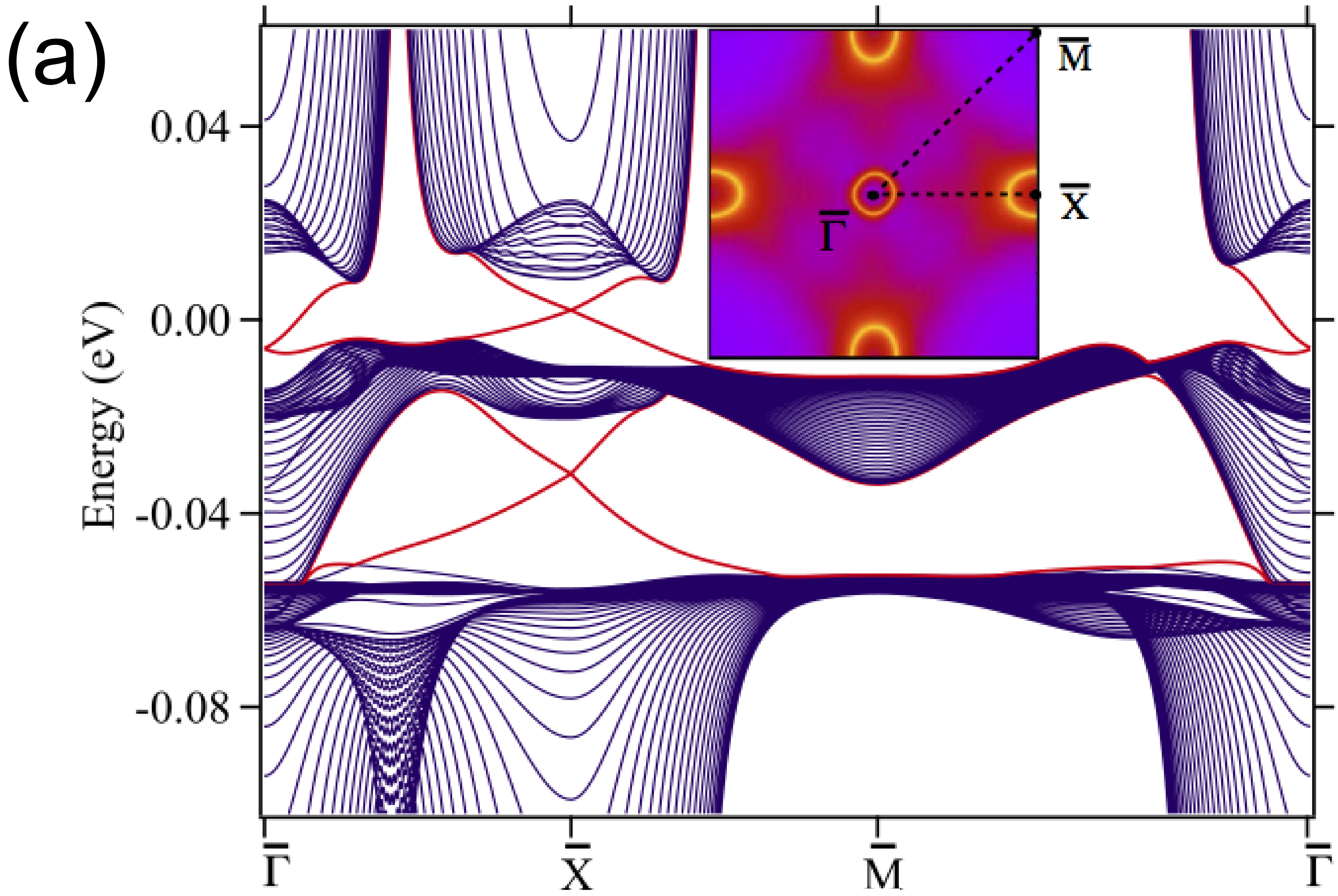
Go to mathematica notebook



$$\mathcal{H}_{jl}(k_x) = \frac{1}{W} \sum_{k_y = \frac{2\pi n}{L}} \exp\left[i k_y (j - l) \right] \underline{h}(k_x, k_y) = a(k)\delta_{jl} + b\delta_{j,l-1} + b^T \delta_{j,l+1}$$

$$a(k_x) = \begin{pmatrix} -2tc_x - \mu & V s_x \\ V s_x & 2tc_x + \lambda \end{pmatrix}, \qquad b = \begin{pmatrix} -t & -V/2 \\ V/2 & t_f \end{pmatrix}$$

Detailed Calculation



Gutzwiller + DFT

F. Lu, et al., Phys. Rev. Lett. 110:096401 (2013)

Three crossings: THREE DIRAC CONES ON SURFACE.

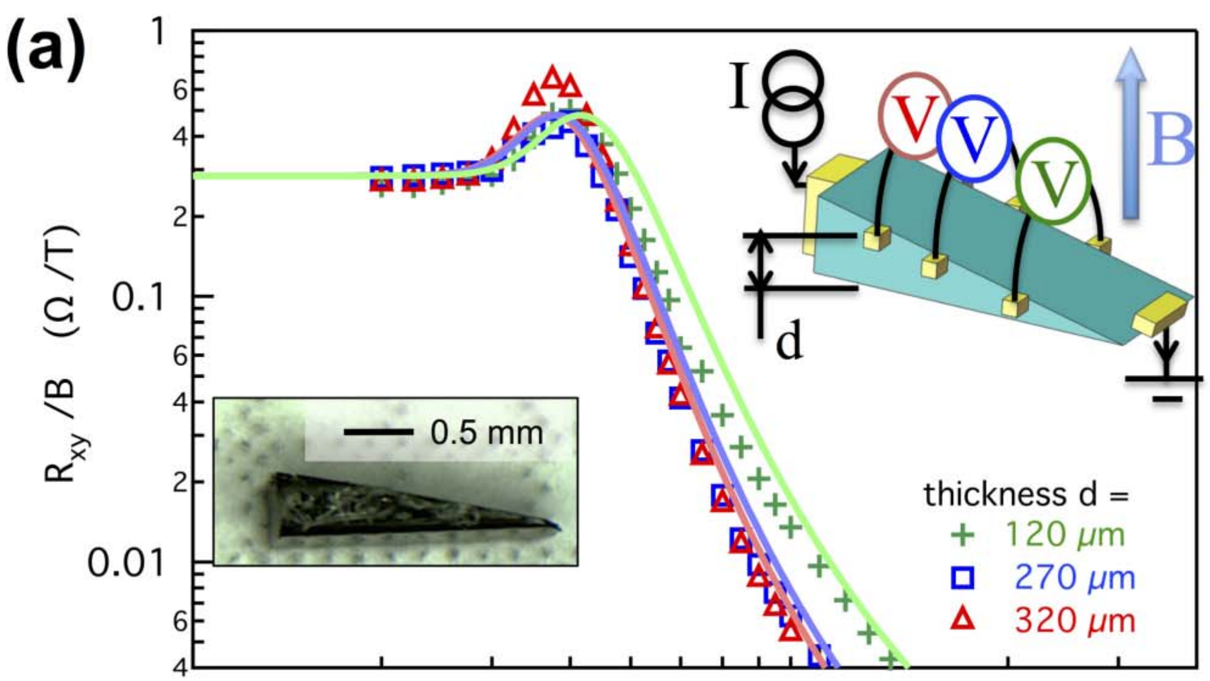
Is SmB6 a topological Kondo insulator?

SmB6 Surface Conductivity

- ☑ Bulk Insulator
- ☑ Surface Conductivity
- ☑ Robustness/Sensitivity to potential/magnetic scattering.

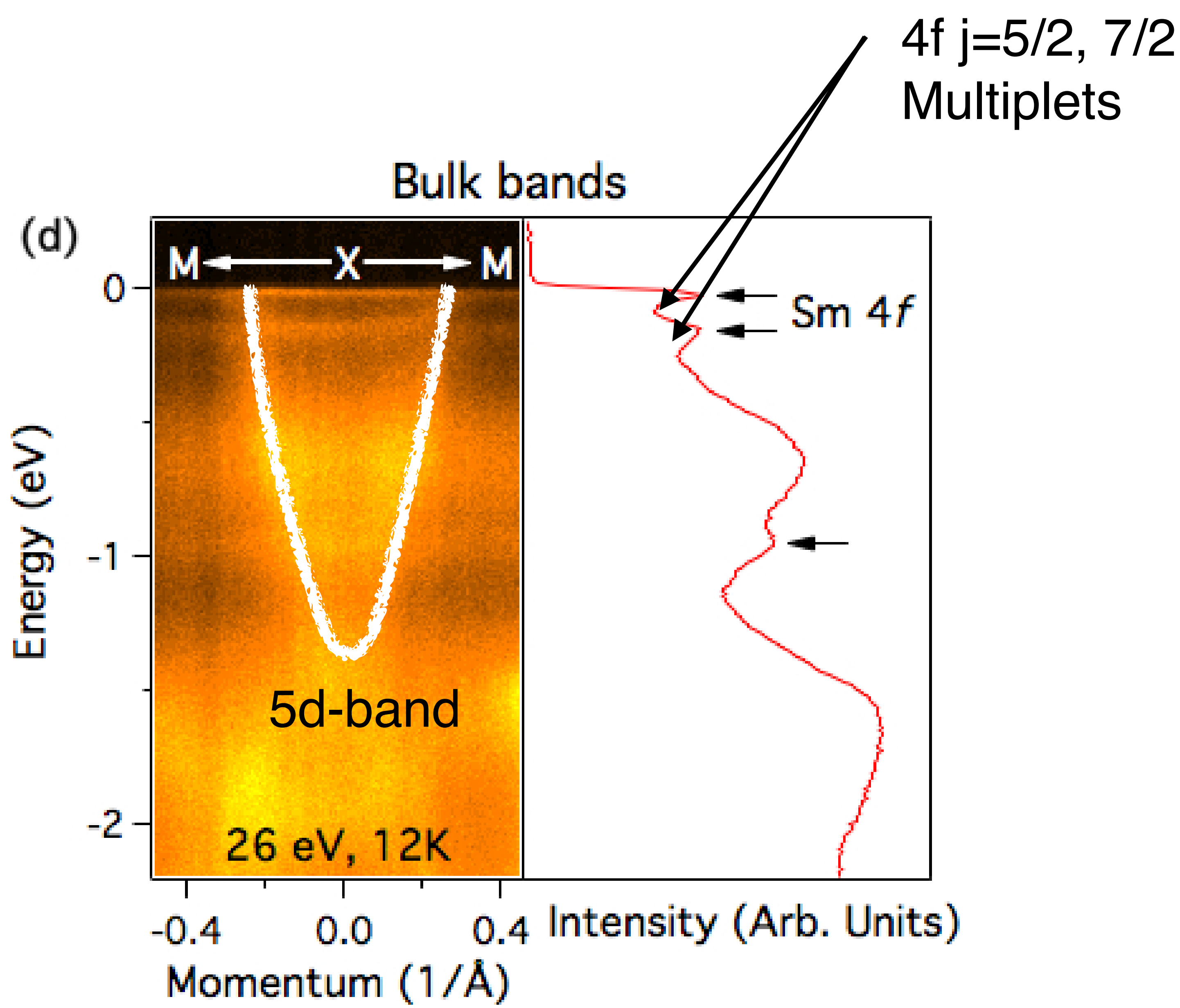
Large Vertical Resistance indicates conductivity is from the surface.

Hall constant derives from the Surface.



D. J. Kim et al, Scientific Reports 3, 3150 (**2013**)

SmB6 ARPES

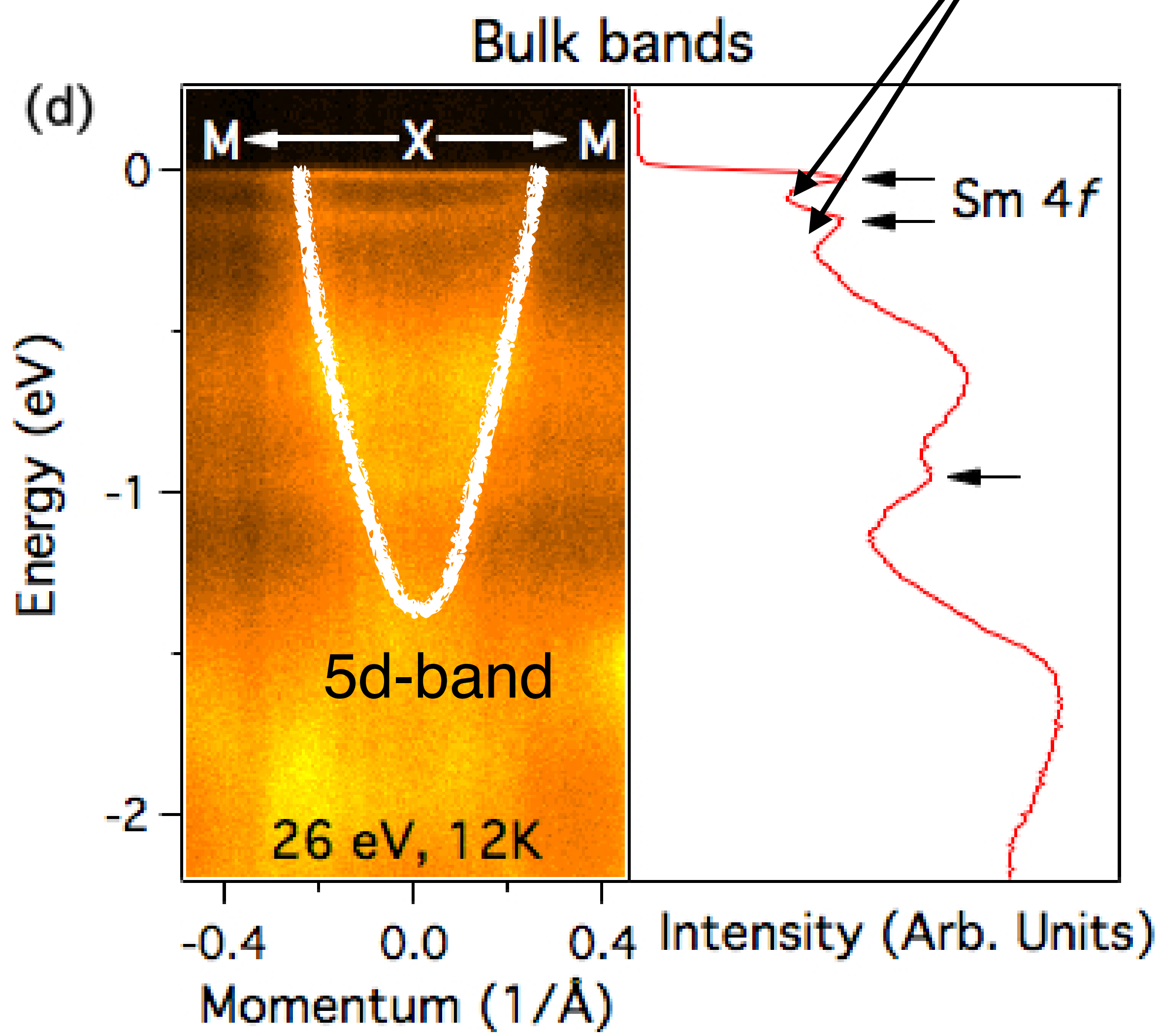


Neupane et al. Nature Commnunications 4, (2013).

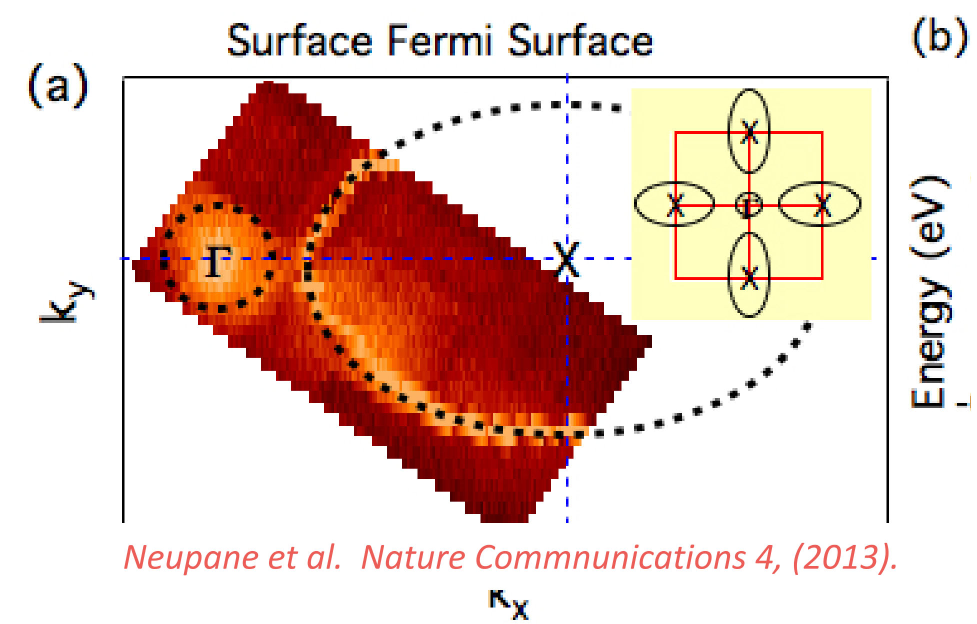
SmB6 ARPES

- ☑ d-band crossing at X points
- ☑ Odd number (3) of Surface FS (ARPES, dHVA, STM).

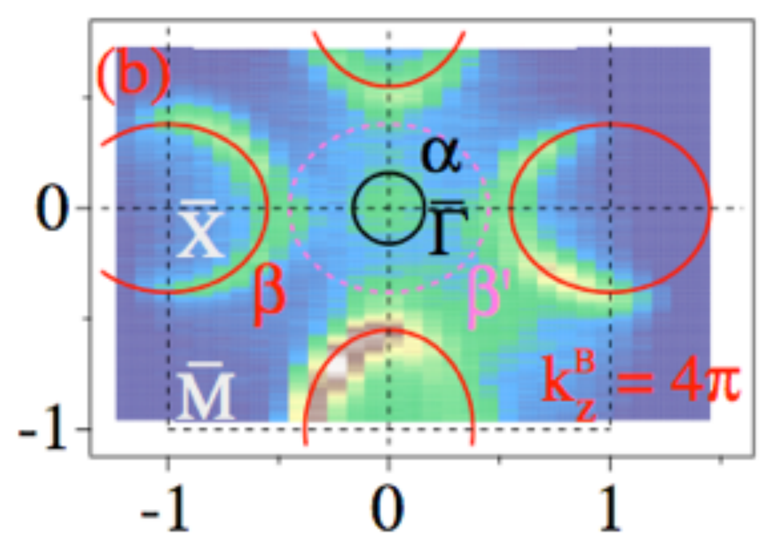
4f j=5/2, 7/2
Multiplets



Neupane et al. Nature Commnunications 4, (2013).



Neupane et al. Nature Commnunications 4, (2013).

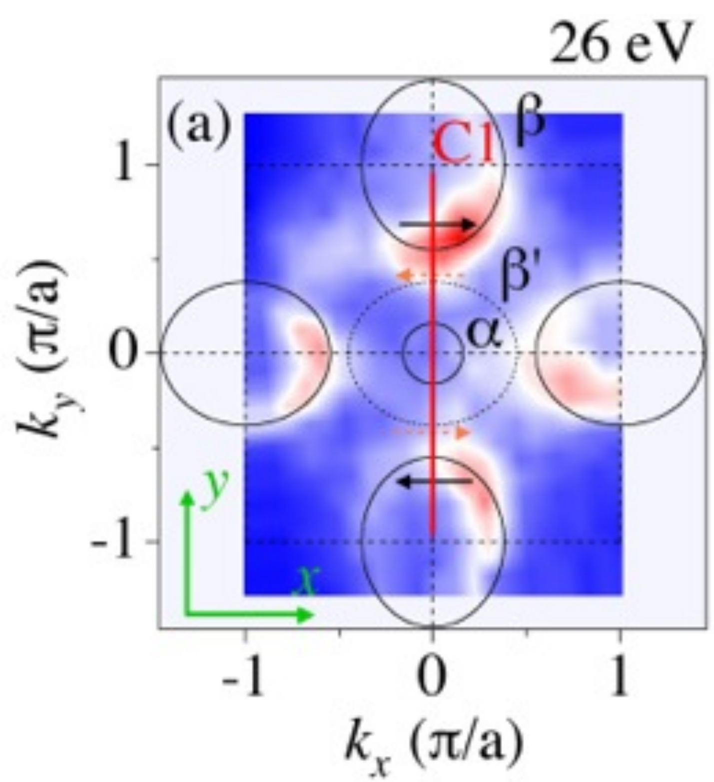


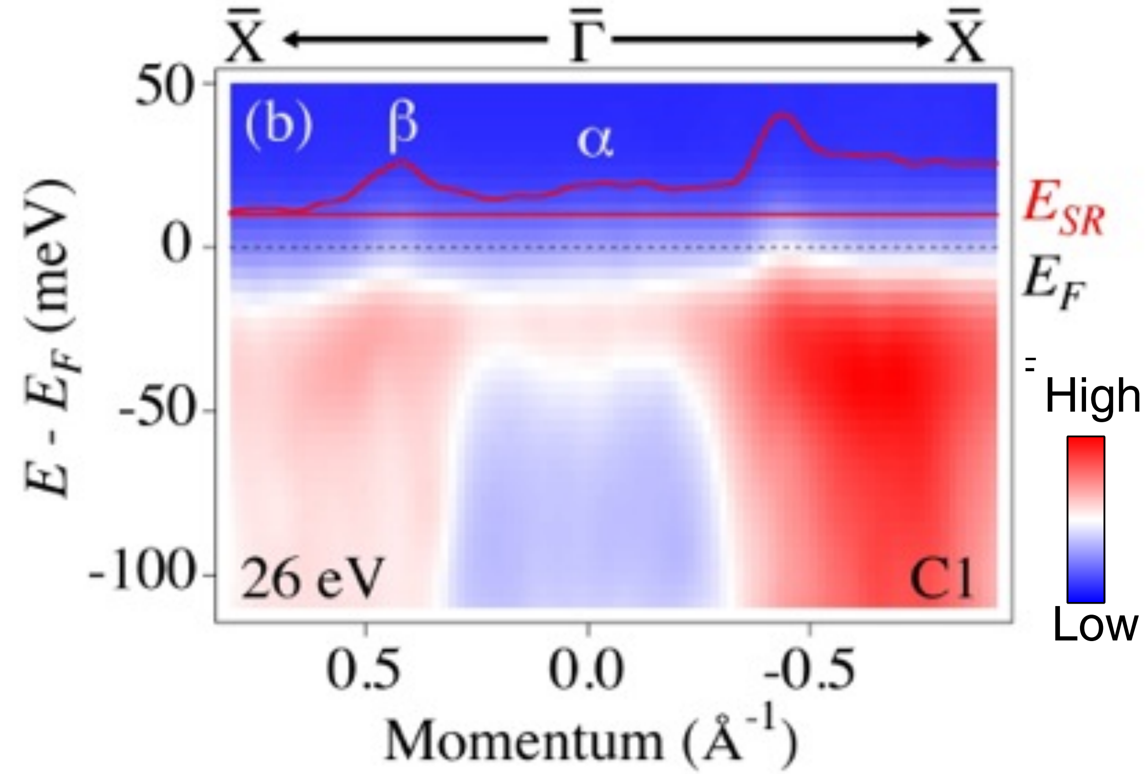
Xu, PRB 88, 121102 (2013)

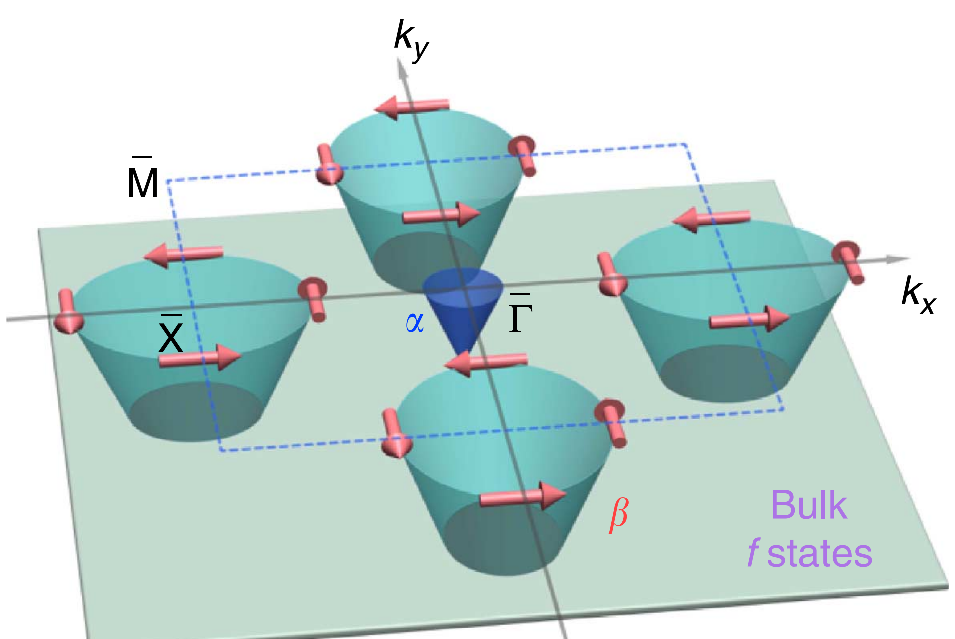
Spin Resolved ARPES

Nan Xu , X. Shi , P. Biswas , C. Matt , R. Dhaka , Y. Huang , N. Plumb , M. Radovic ,
J. Dil , E. Pomjakushina , K. Conder , A. Amato , Z. Salman , D. Paul , J. Mesot , Hong Ding , Ming Shi

Nature Communications Volume: 5, 4566 (2014)







But no consensus yet!

Phys. Rev. Lett. 111, 216402 (2013)

Polarity-Driven Surface Metallicity in SmB_6

Z.-H. Zhu,[1] A. Nicolaou,[1,2] G. Levy,[1,2] N. P. Butch,[3] P. Syers,[3] X. F. Wang,[3]
J. Paglione,[3] G. A. Sawatzky,[1,2] I. S. Elfimov,[1,2,*] and A. Damascelli[1,2,†]

arxiv/1502.01542

Samarium hexaboride: A trivial surface conductor

P. Hlawenka,[1] K. Siemensmeyer,[1] E. Weschke,[1] A. Varykhalov,[1] J. Sánchez-Barriga,[1] N. Y. Shitsevalova,[2]
A. V. Dukhnenko,[2] V. B. Filipov,[2] S. Gabáni,[3] K. Flachbart,[3] O. Rader,[1] and E. D. L. Rienks[1]

[1]Helmholtz-Zentrum Berlin für Materialien und Energie,
Elektronenspeicherring BESSY II, Albert-Einstein-Straße 15, 12489 Berlin, Germany
[2]Institute for Problems of Materials Science, National Academy of
Sciences of Ukraine, Krzhyzhanovsky str. 3, 03142 Kiev, Ukraine

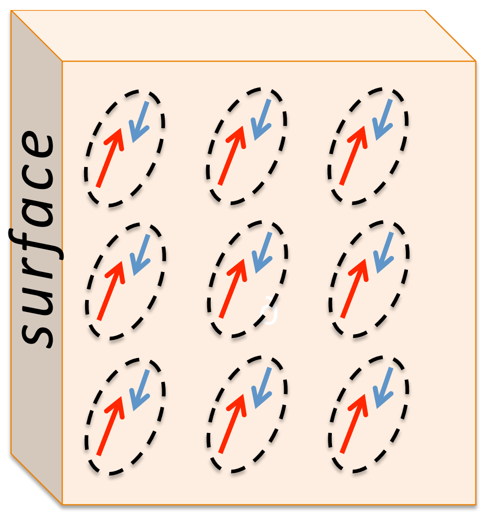
The magnetic connection.

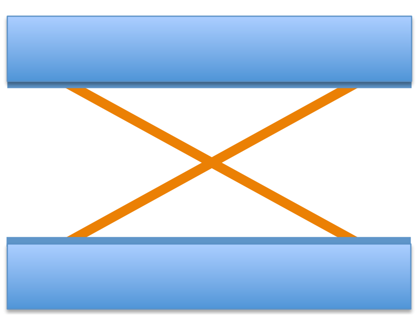
I. Kondo Breakdown
II. Pressure:AFM
III. Neutrons: Exciton
IV. Field: dHvA and Quantum Criticality.

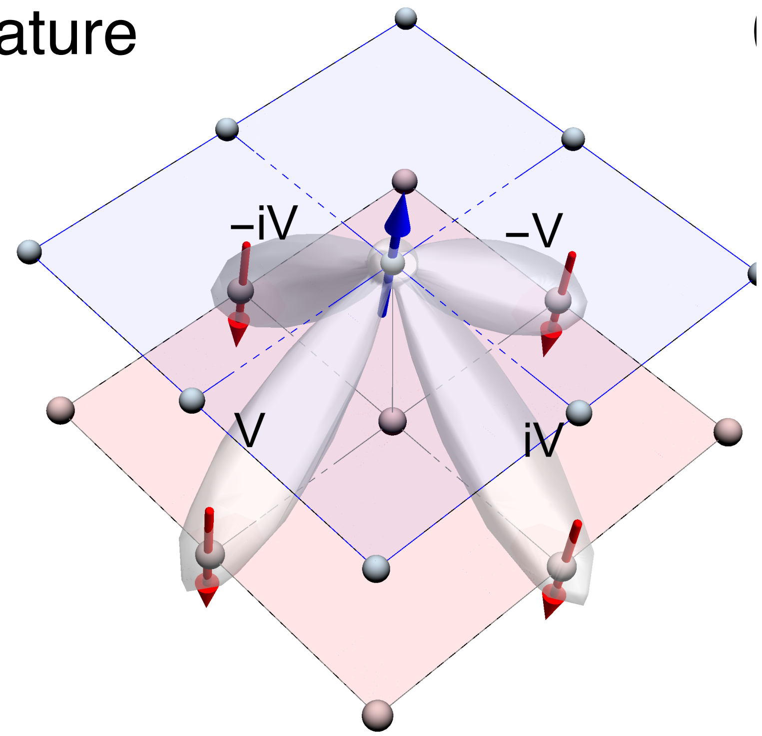
I. Kondo Breakdown

V. Alexandrov, P. Coleman, O. Erten,
Phys. Rev. Lett. 114:177202 2015.

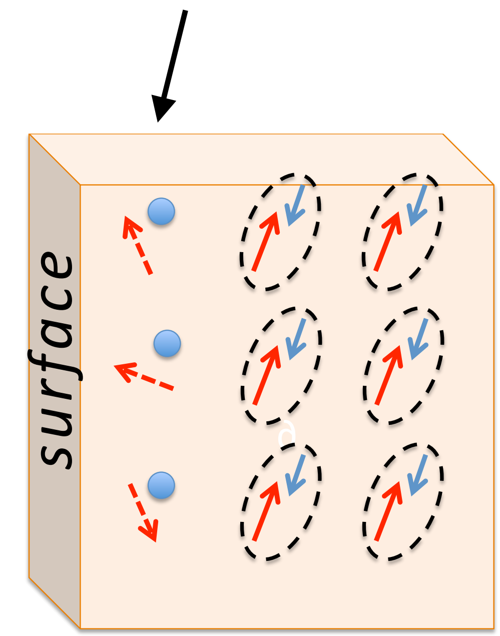
Lower co-ordination at surface dramatically suppresses the Kondo temperature







Kondo Breakdown at surface.



ARPES: $v_s \sim$ 220-300 meVA

Theory: $v_s \sim$ 30-50 meVA

10x too small!

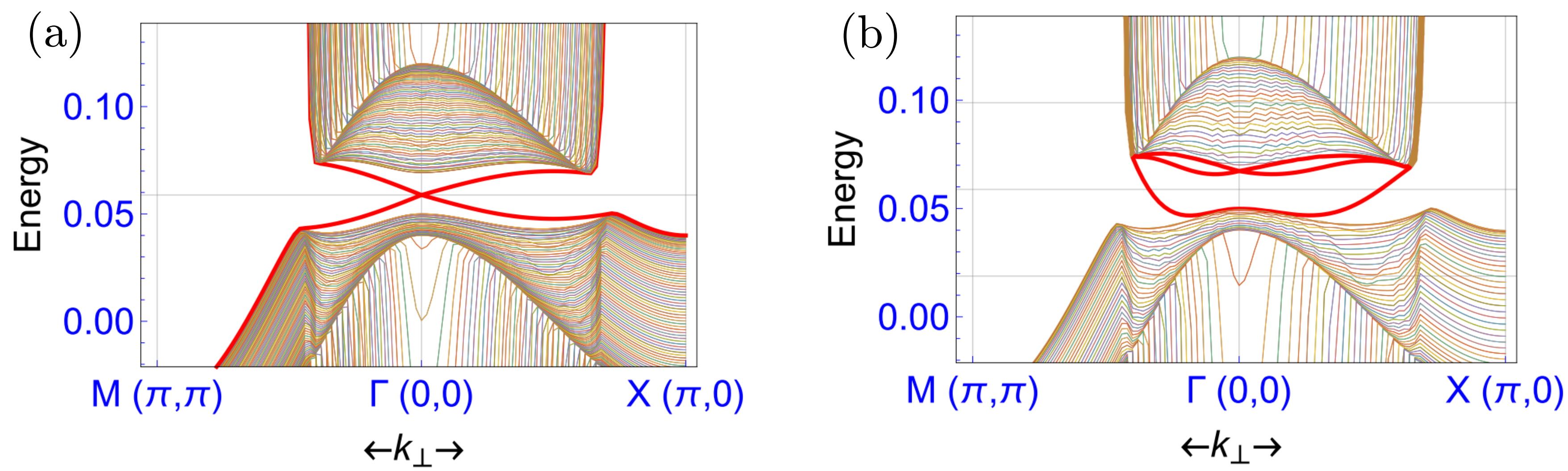
$$\mathcal{A}_{\rm FS}/(2\pi)^2 = \Delta n_f$$

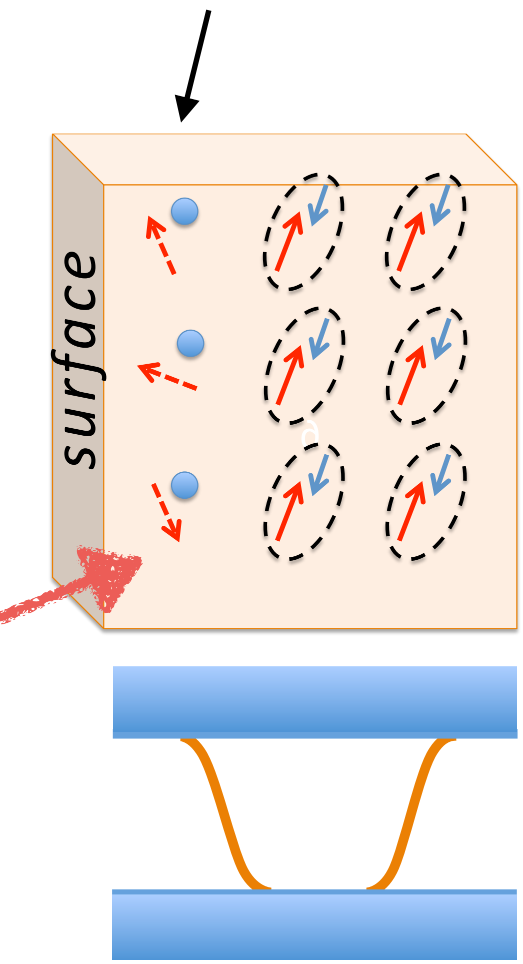
Breakdown of Kondo effect at surface causes surface Dirac cones to dope, submerging the Dirac point and considerably enhancing the Fermi velocity.

I. Kondo Breakdown

V. Alexandrov, P. Coleman, O. Erten,
Phys. Rev. Lett. 114:177202 2015.

Kondo Breakdown at surface.





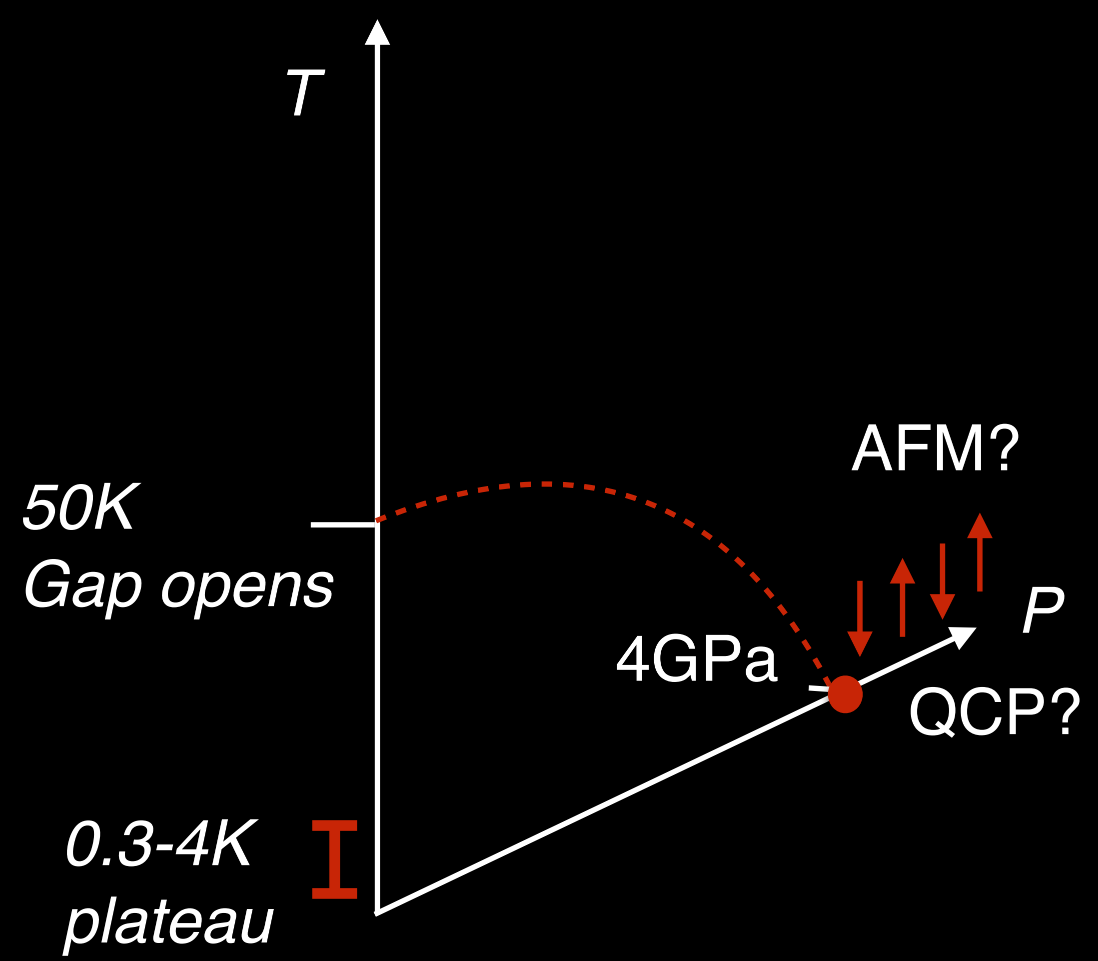
Local moments on the surface form a 2D Kondo lattice with spin-orbit locked conduction bands.

Surface Kondo physics? Magnetism, QCP even superconductivity.

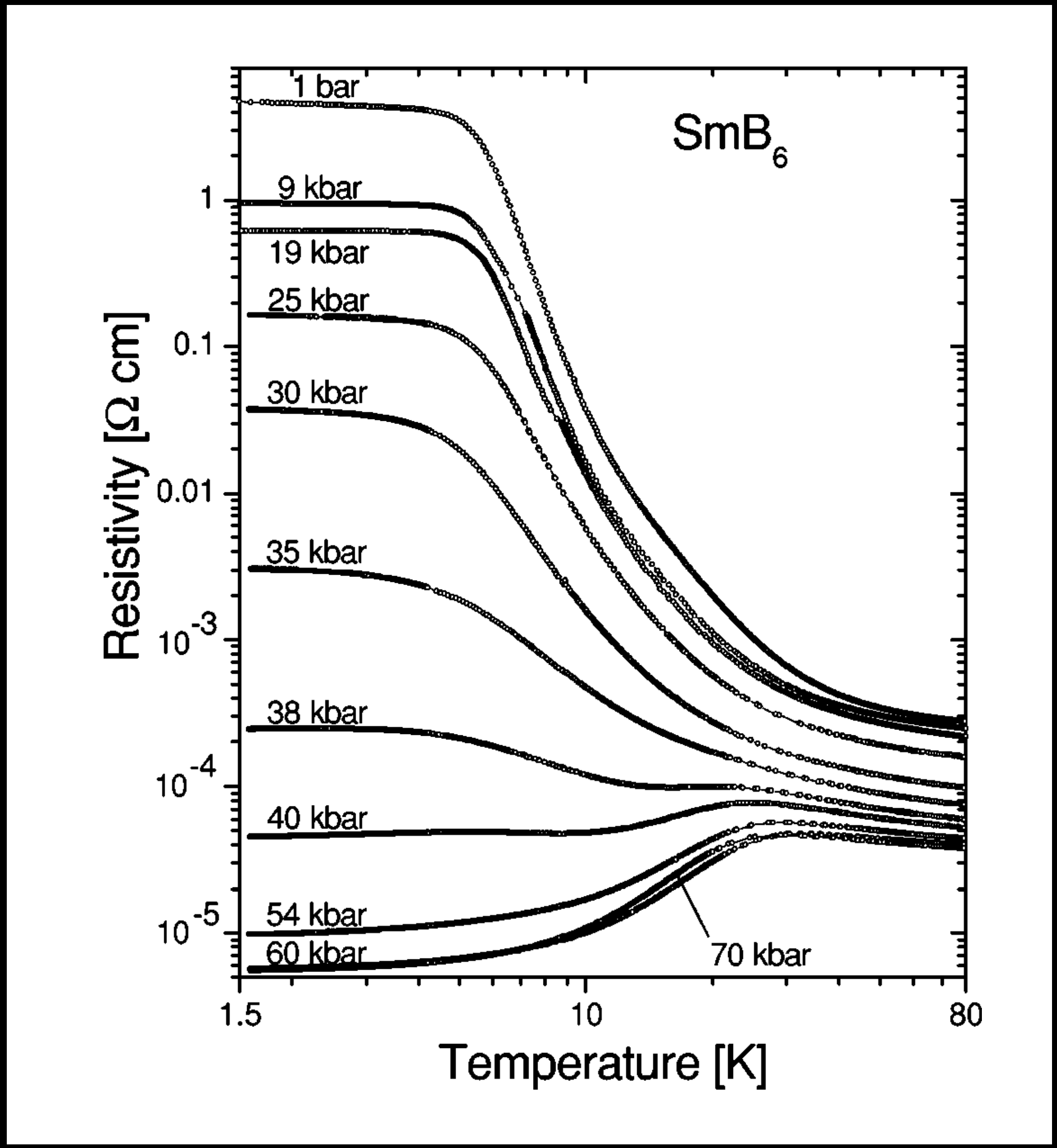
$$\mathcal{A}_{\rm FS}/(2\pi)^2 = \Delta n_f$$

Breakdown of Kondo effect at surface causes surface Dirac cones to dope, submerging the Dirac point and considerably enhancing the Fermi velocity.

II. The effect of Pressure: AFM



S. Gabani et al, PRB 67, 172406 (2003)



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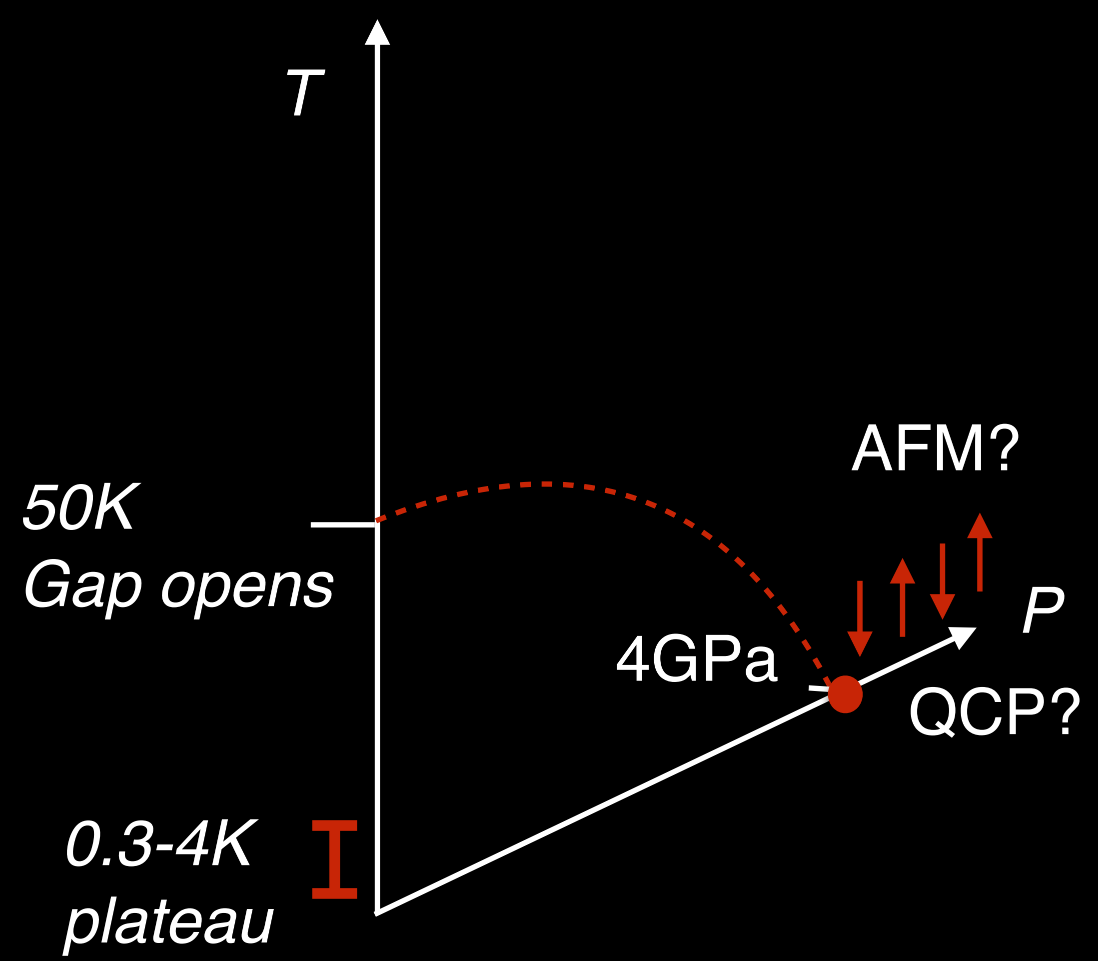
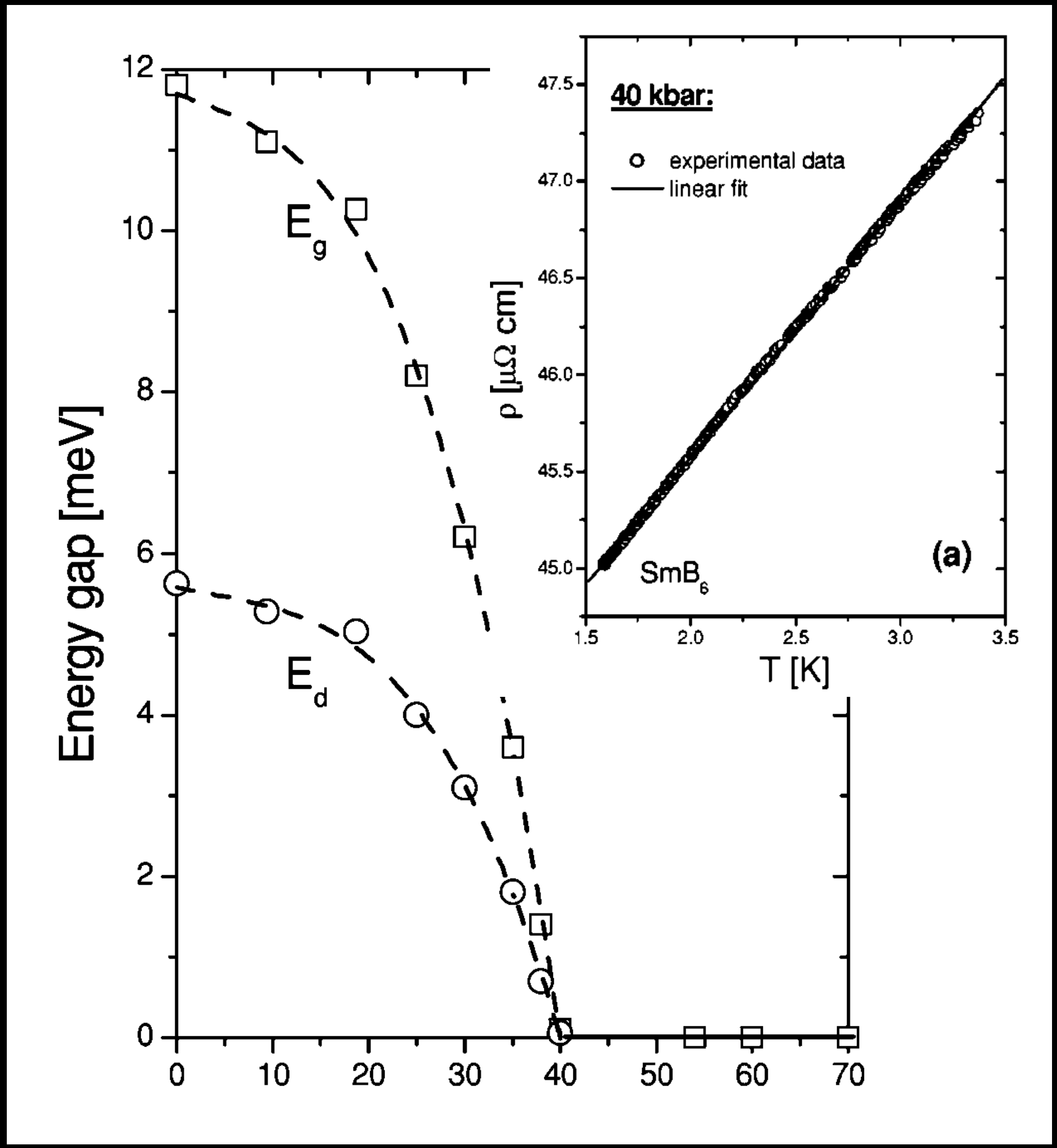


S. Gabani et al, PRB 67, 172406 (2003)



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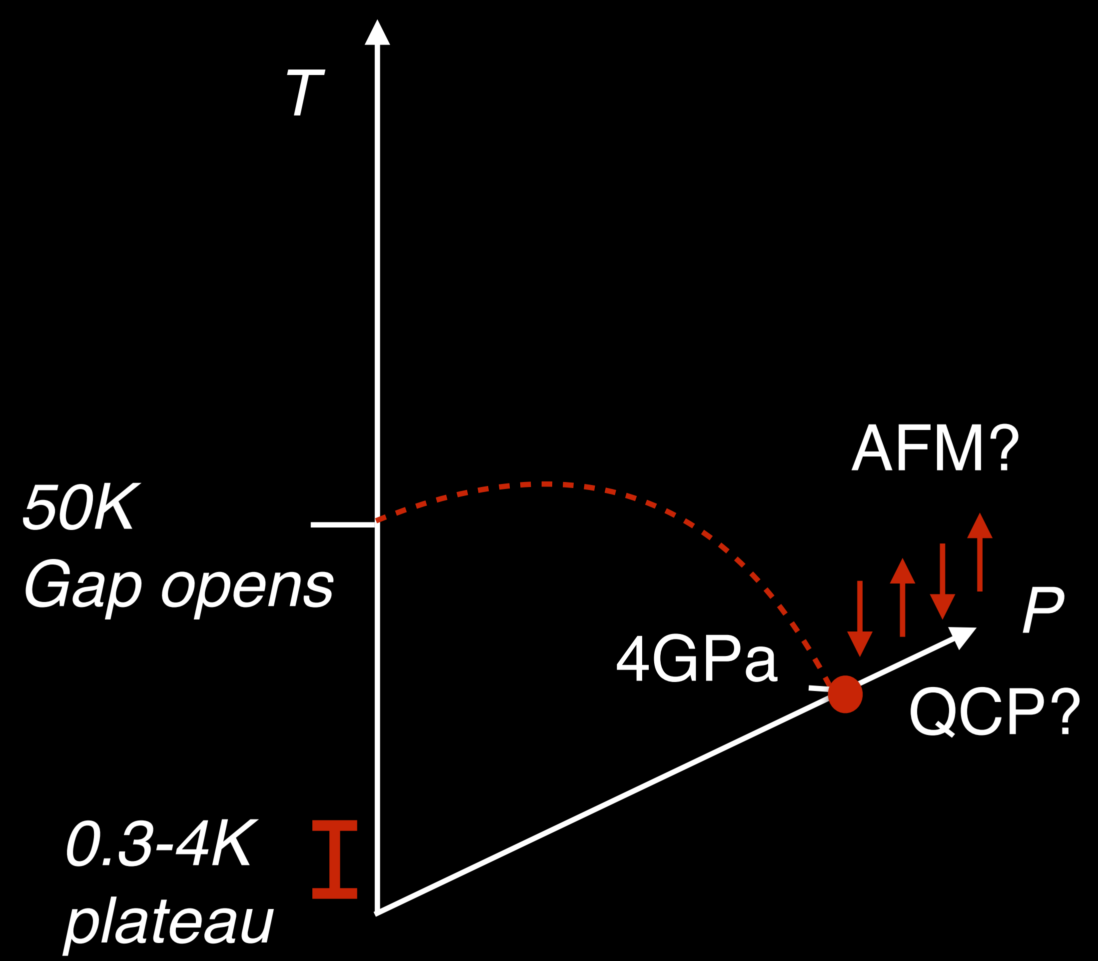
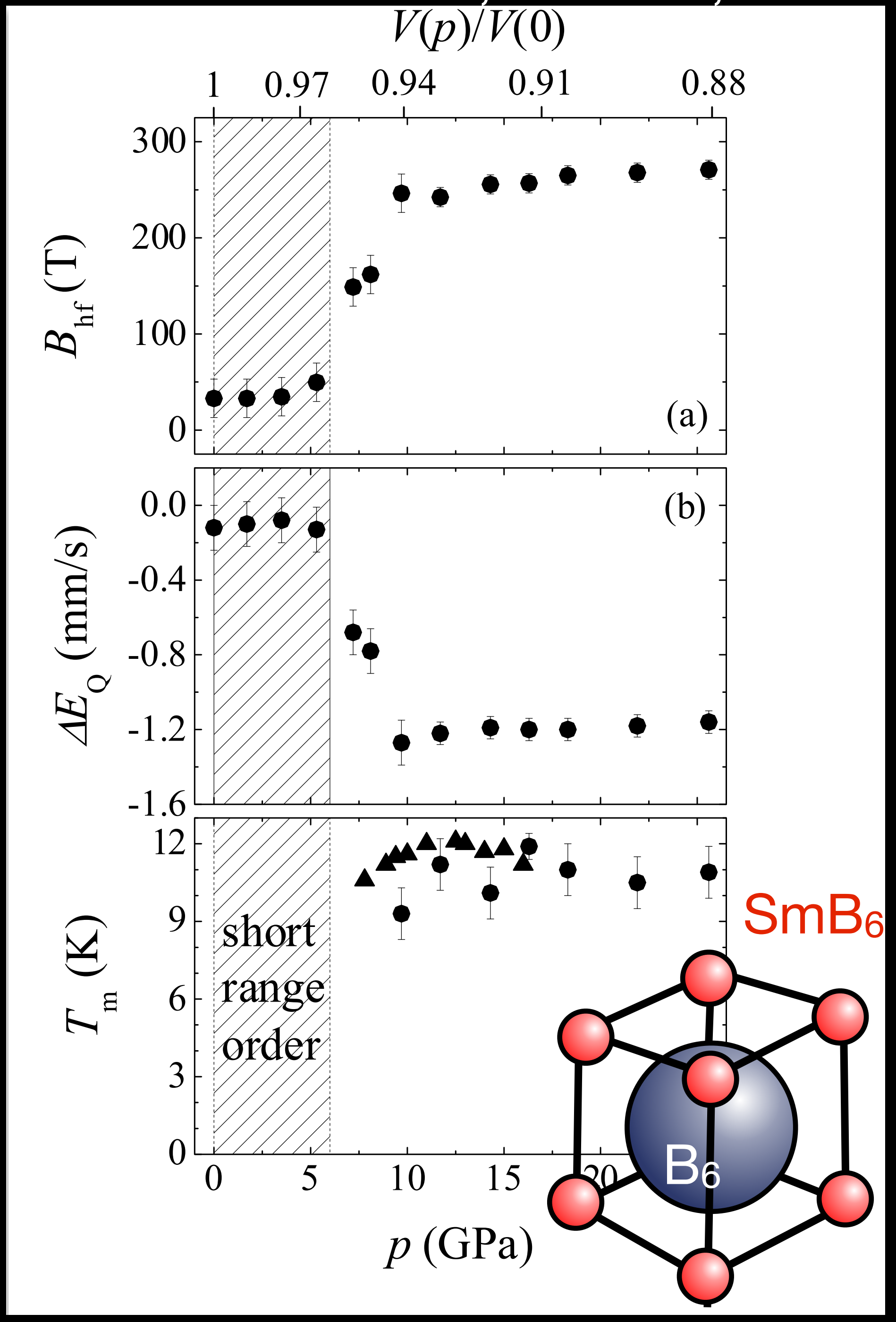
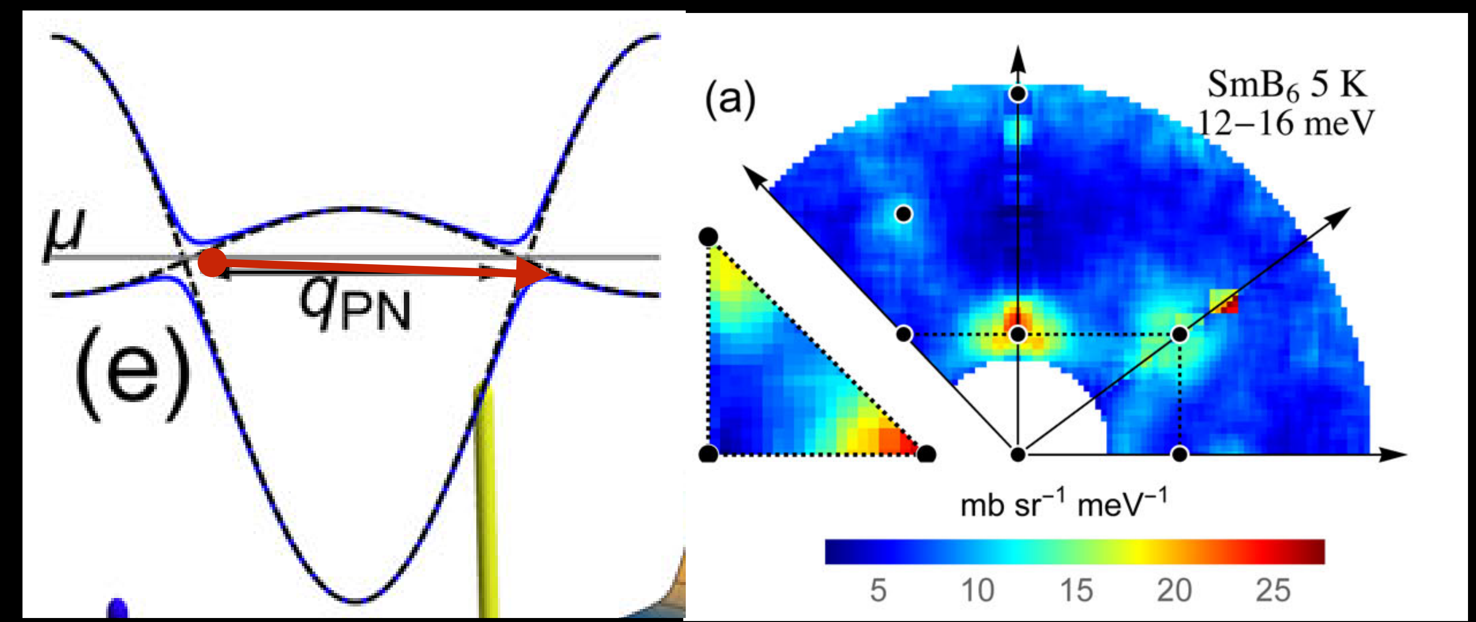


A. Barla et al, PRL 94, 2005

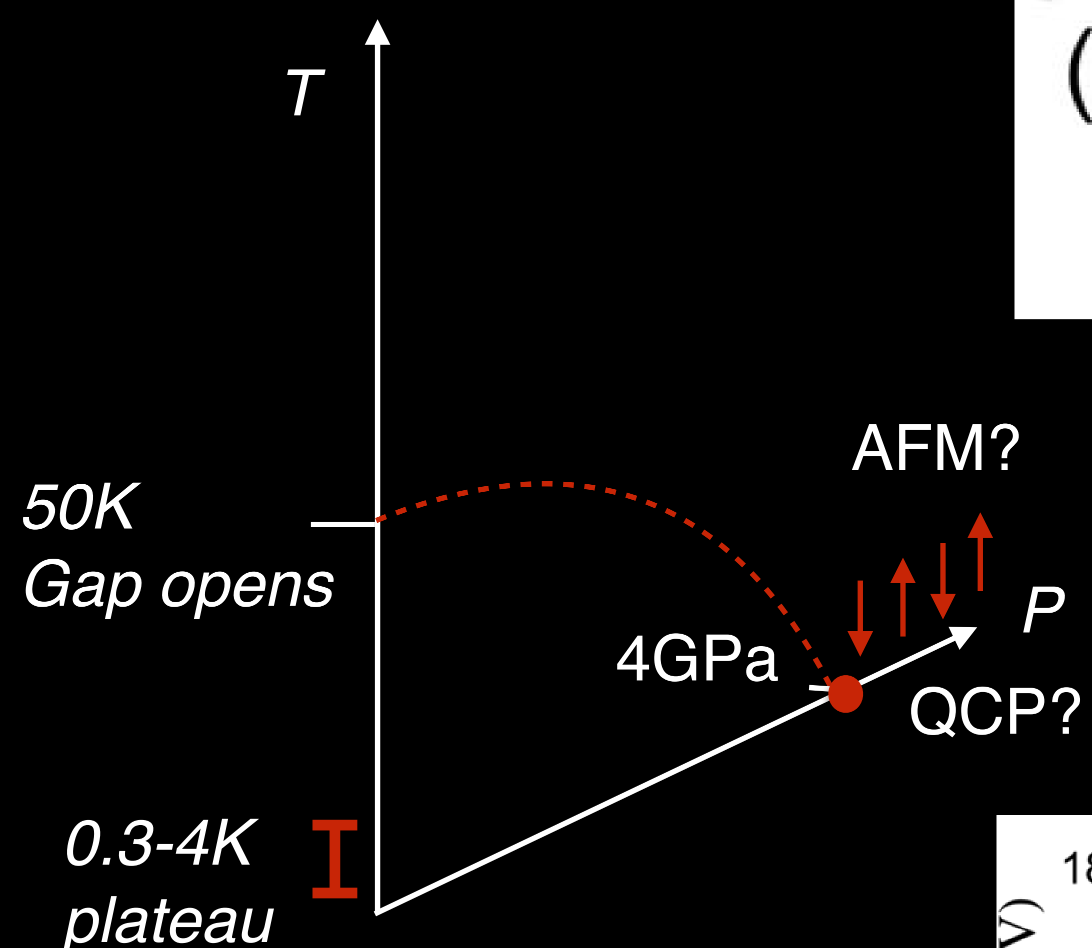


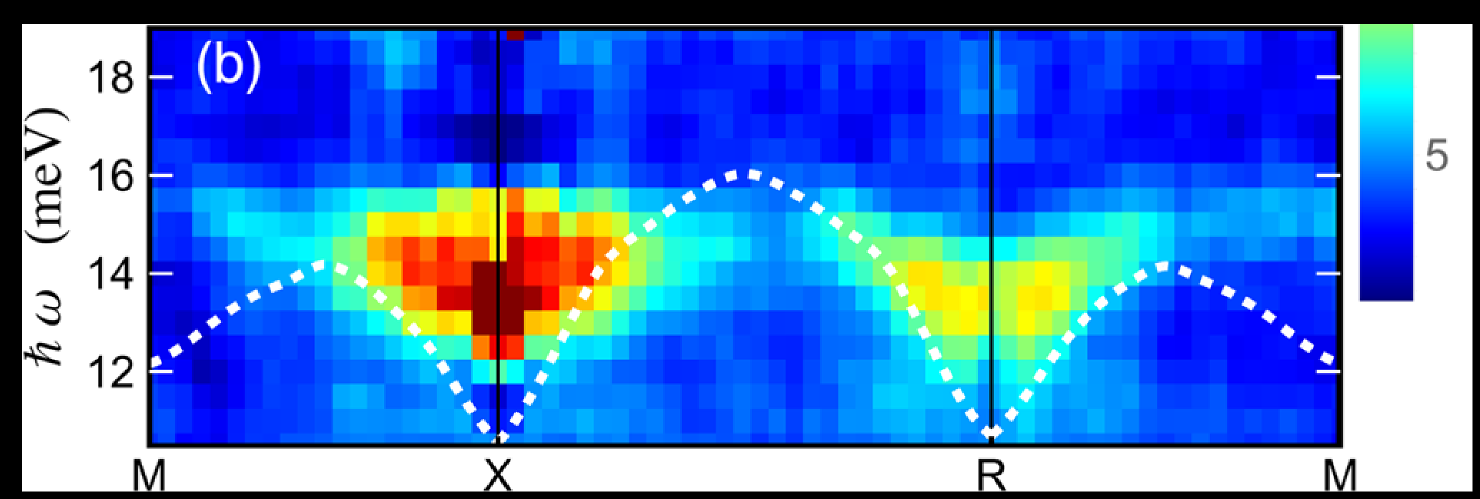
III. Magnetic Fluctuations

Fuhrman et al, PRL 114, 036401 (2015)



AFM Fluctuations





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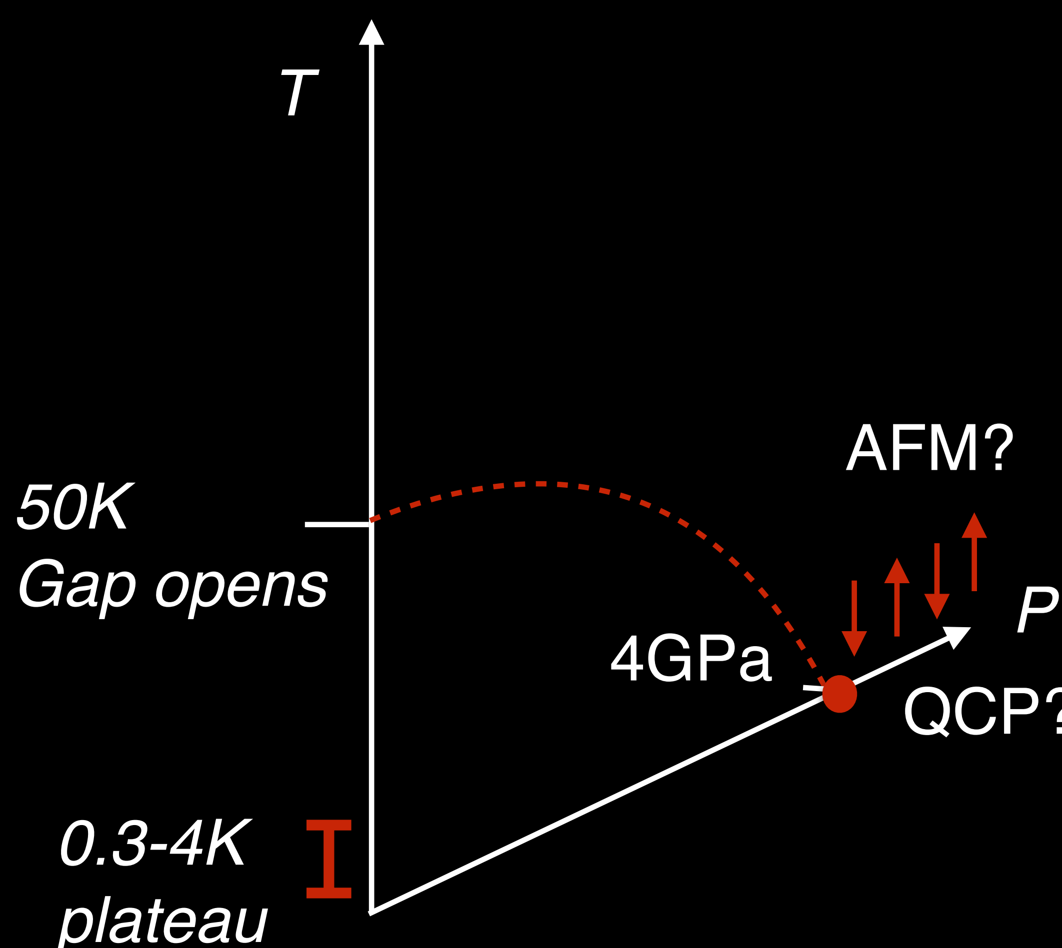
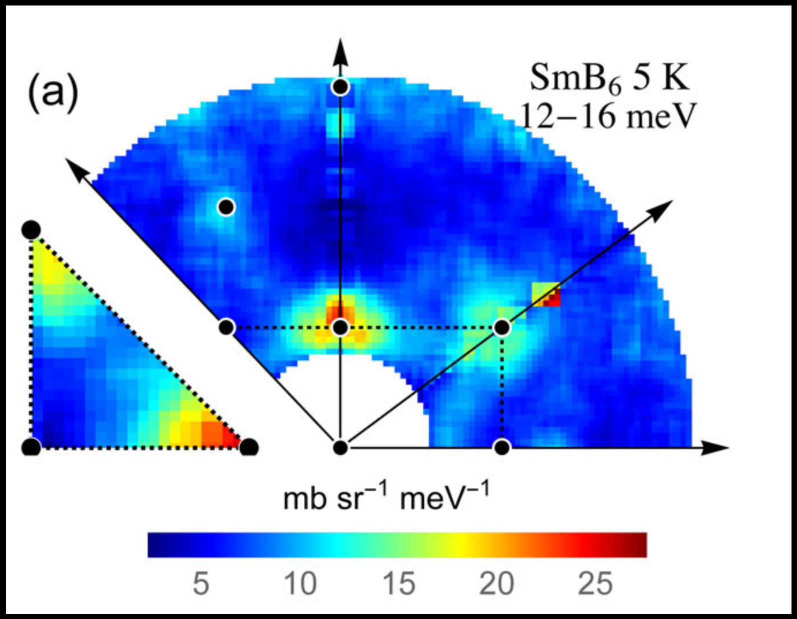
Fuhrman et al, PRL 114, 036401 (2015)





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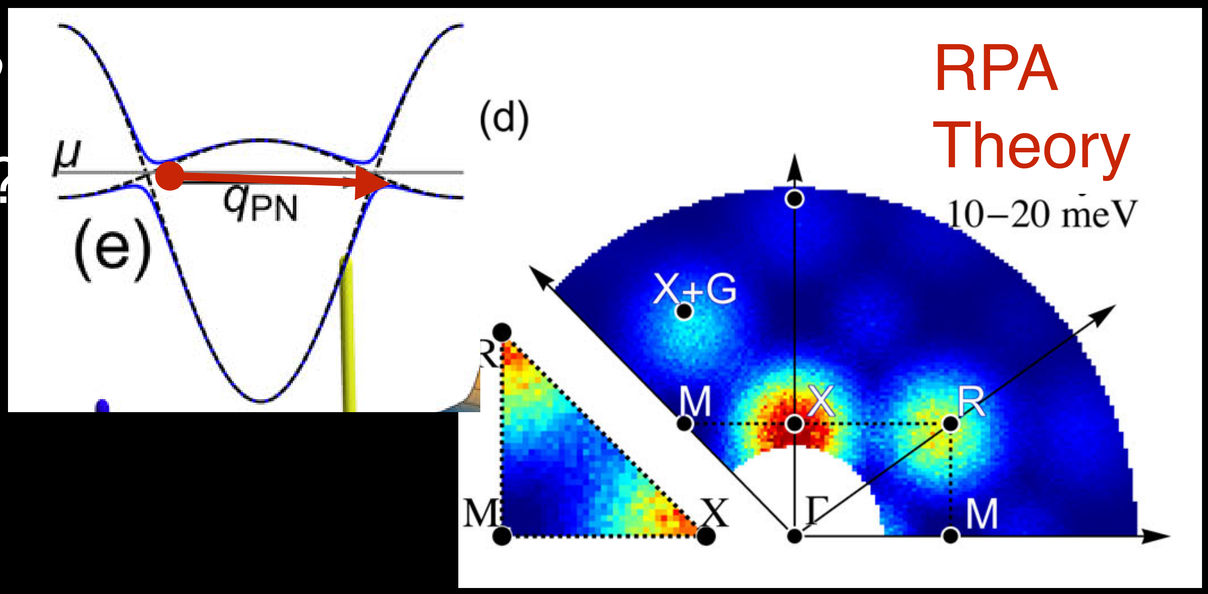
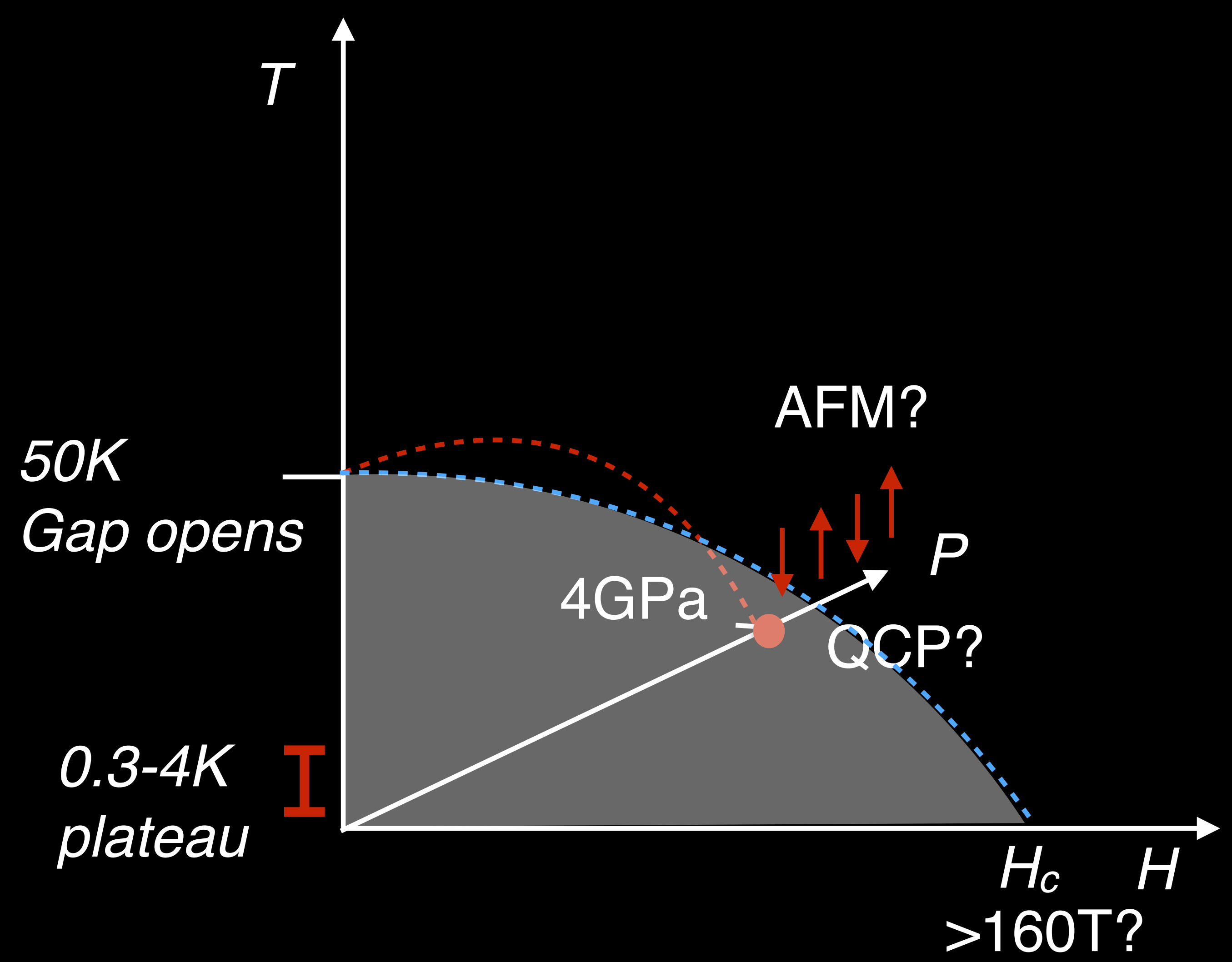
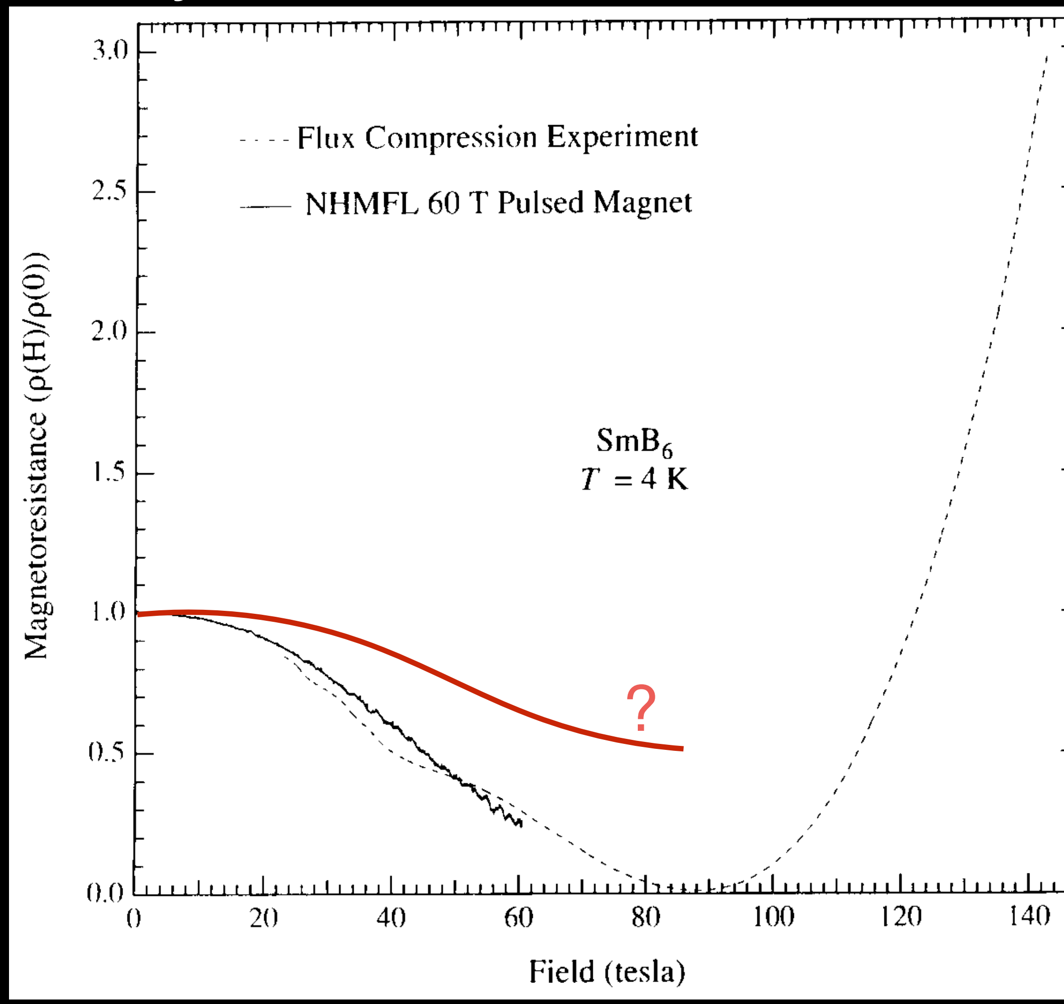


IV. Field effect



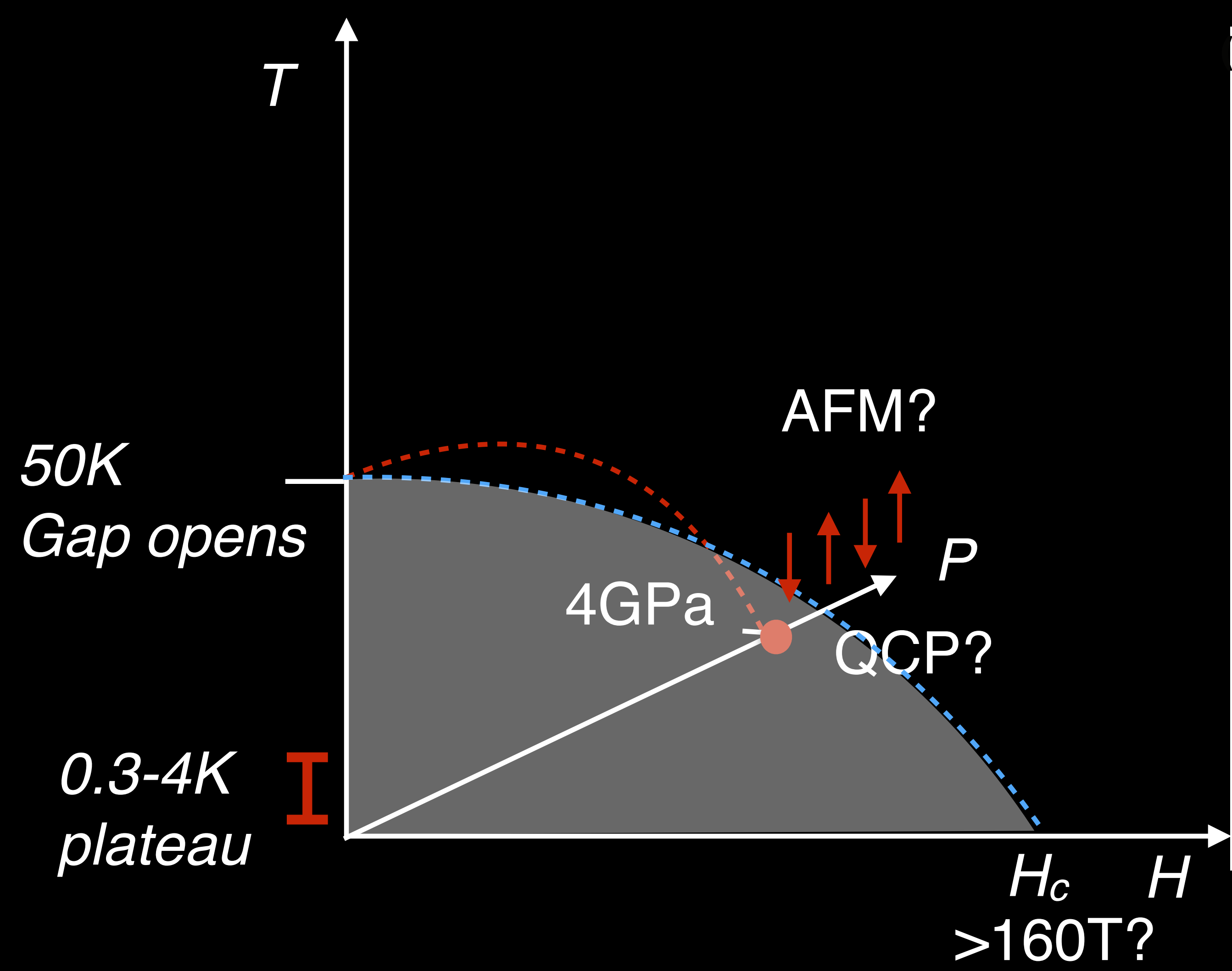
Cooley et al, 1999



L=5, S=5/2, J=5/2, g~0.2-0.3

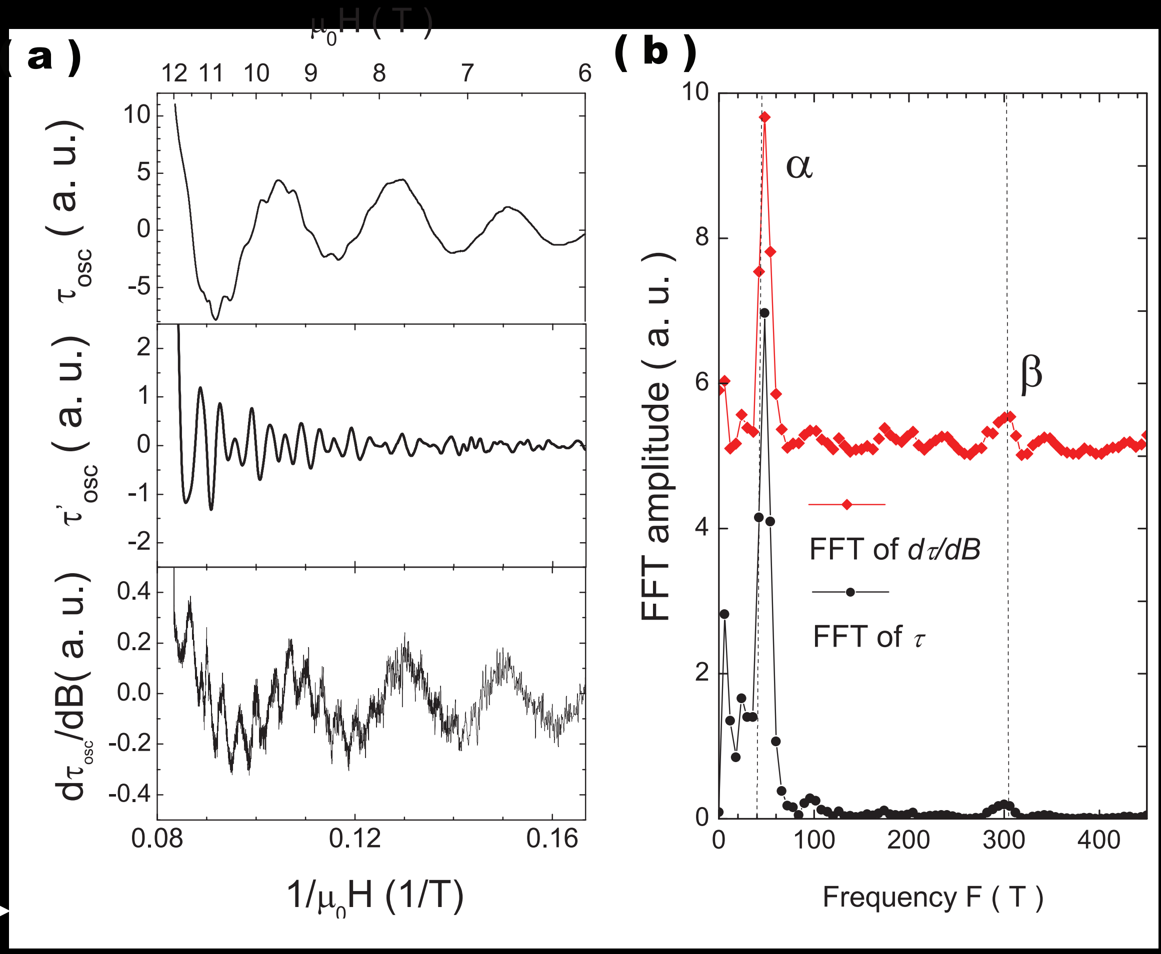
Field effect is *ORBITAL*

IV. Field effect



2D fluctuations:

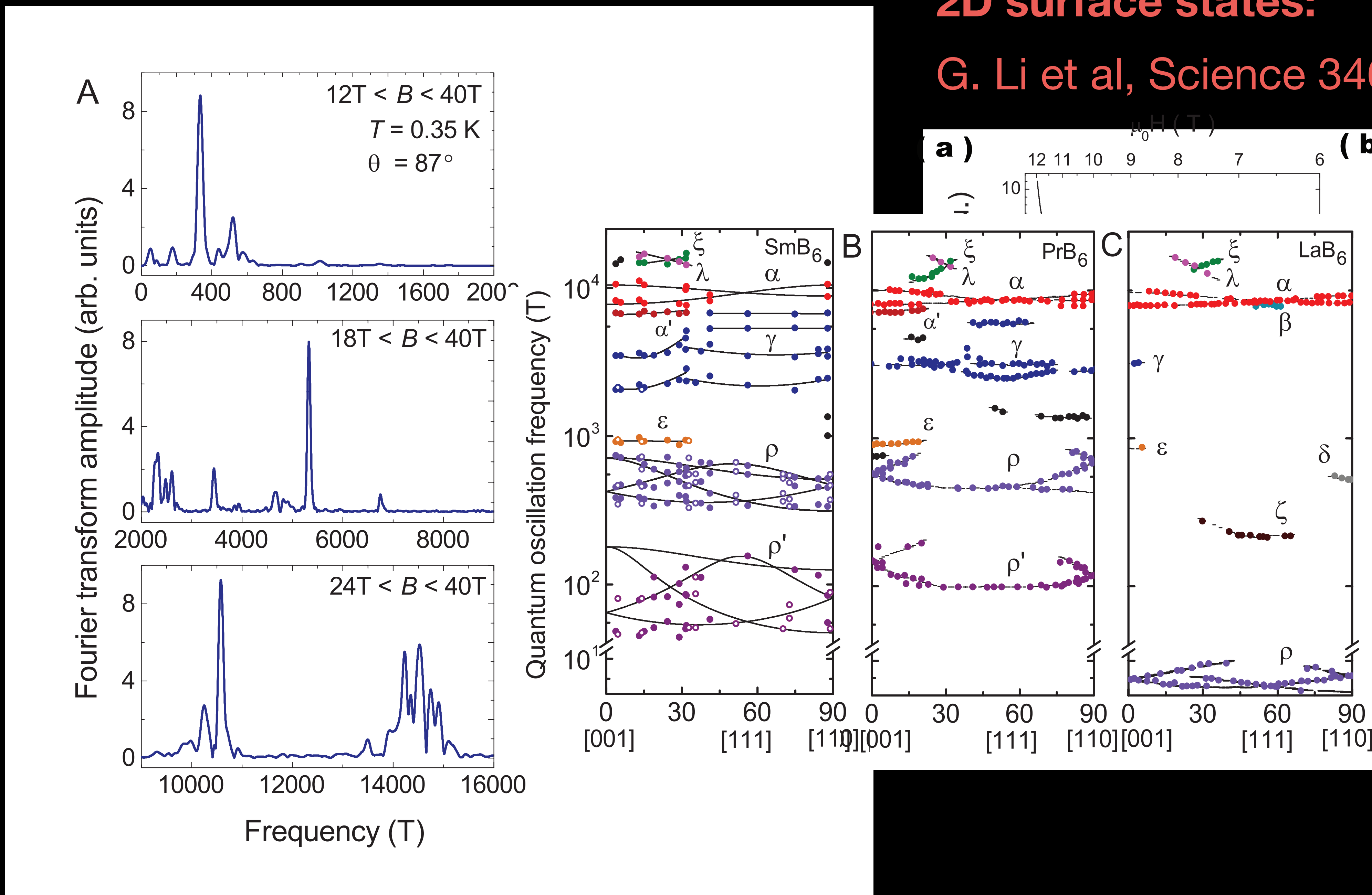
G. Li et al, Science 346, 1208 (2014).



IV. Field effect

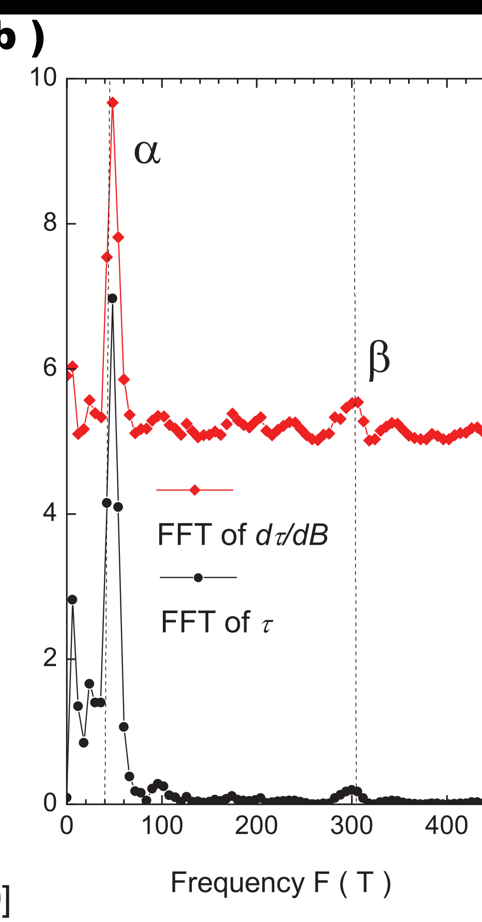
3D orbits!

Tan et al, Science (2015).



2D surface states:

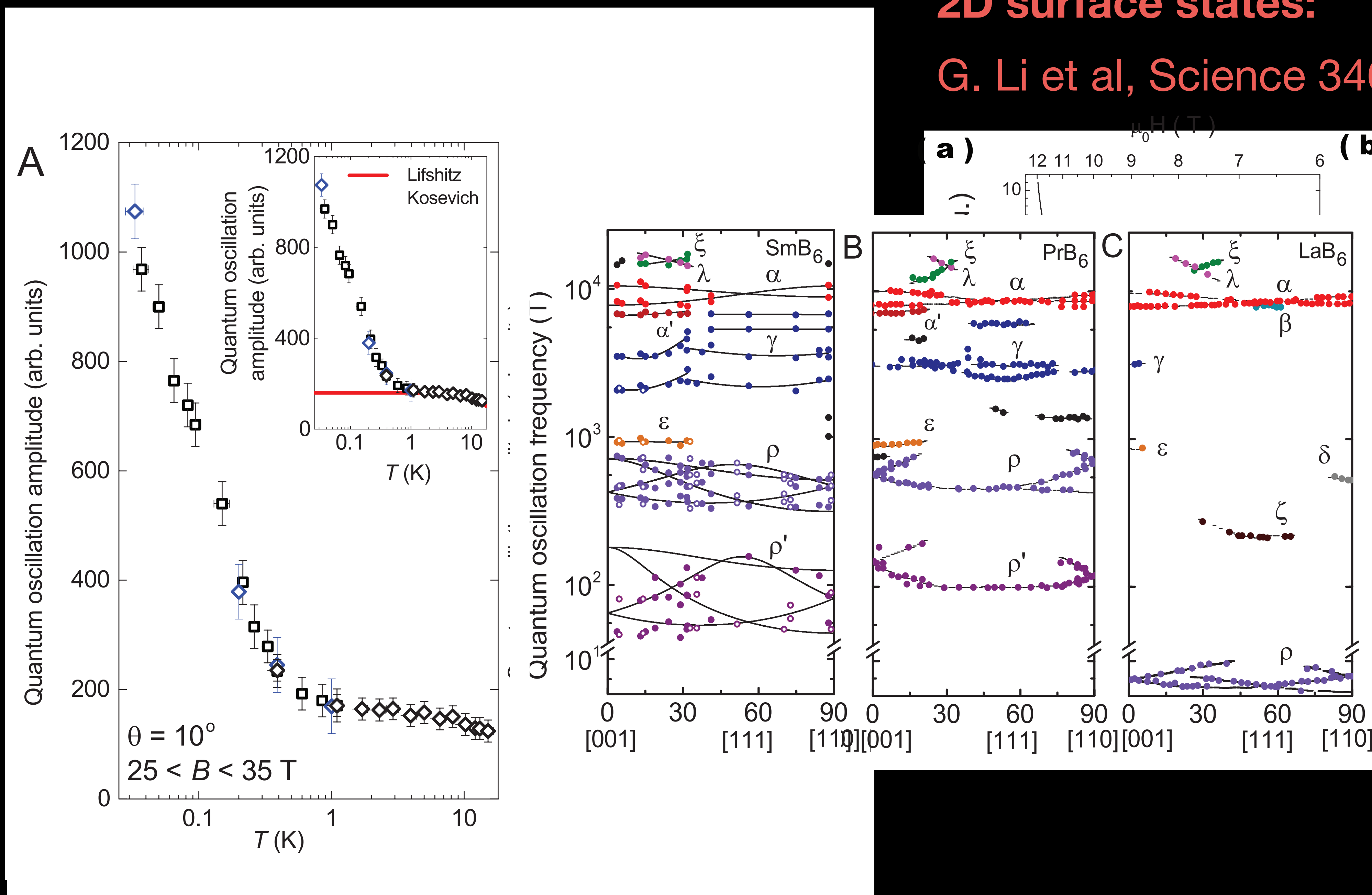
G. Li et al, Science 346, 1208 (2014).



IV. Field effect

3D orbits! **6x Rise in N(0)*: Q Criticality?**

Tan et al, Science (2015).



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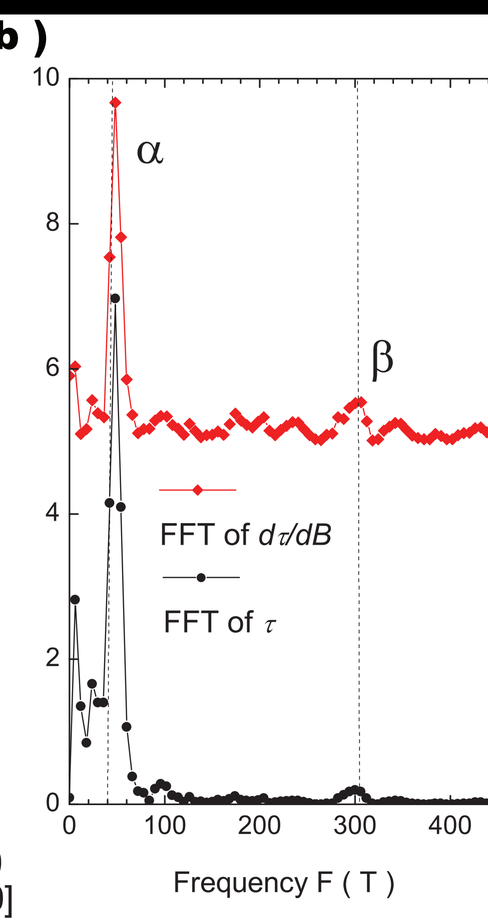

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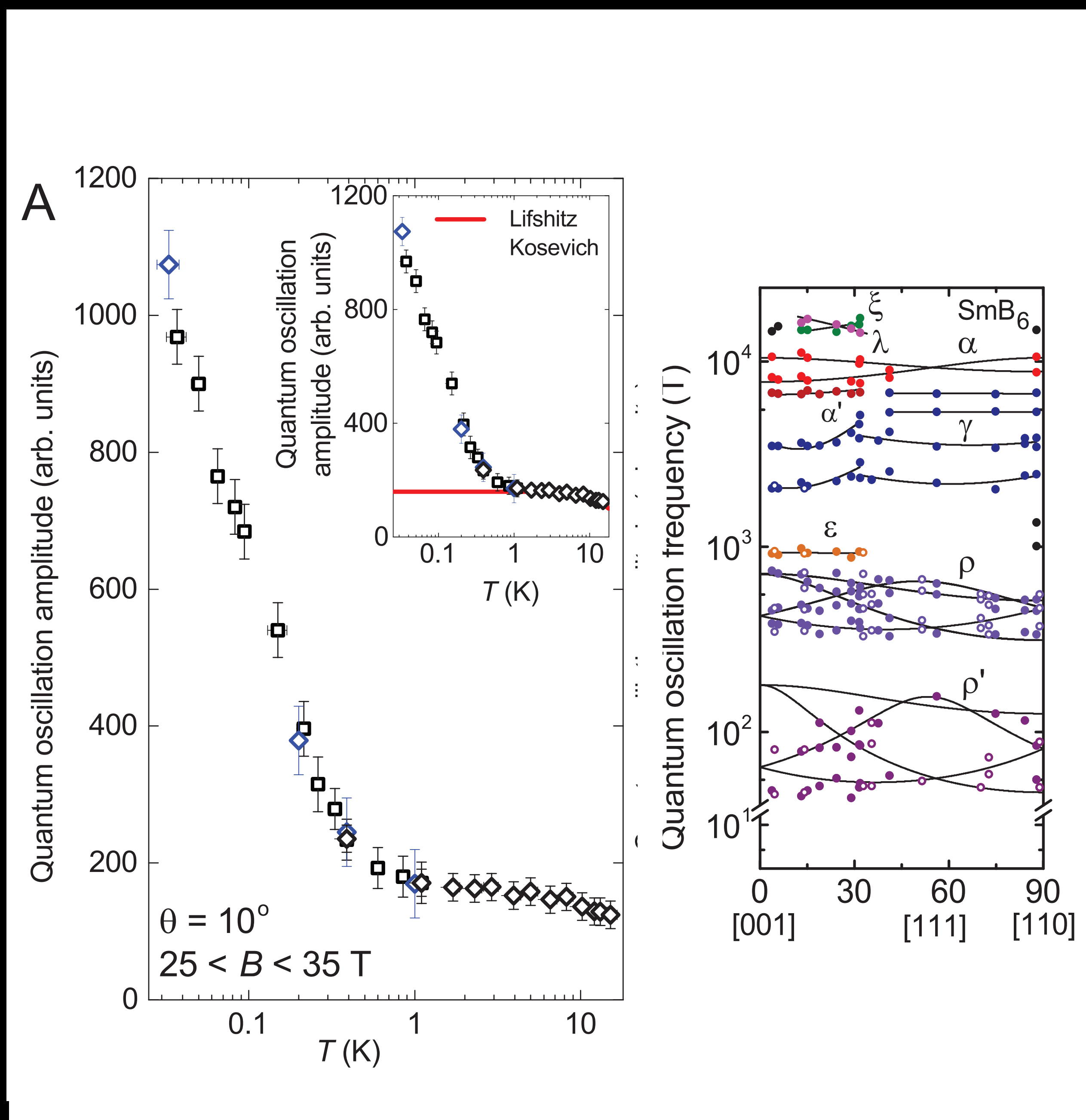
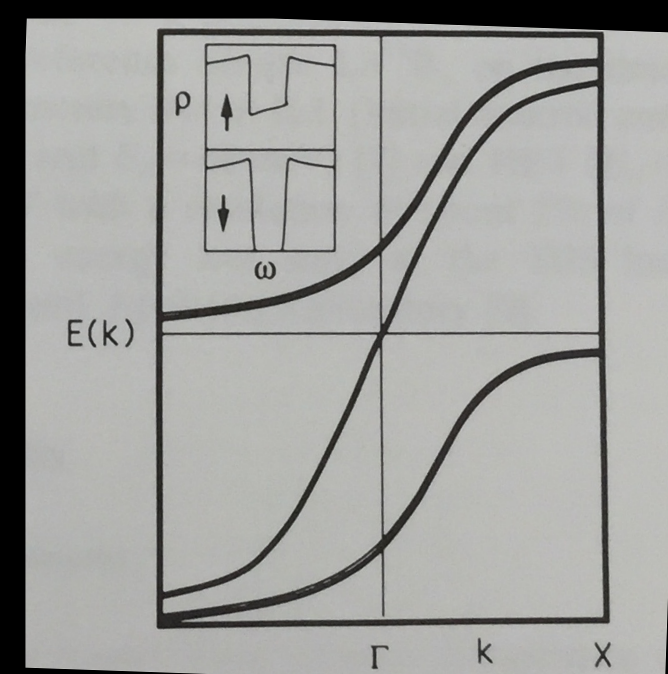


- 3D FS in a bulk insulator !
- $\omega_c \gtrsim$ **V ?**

  (Knolle &Cooper arXiv 1507.00885)
- Majorana FS? Are KI gapless?

  (Baskaran arXiv 1507.03477; see also Miranda, PC, Tsvelik, Physica B, 186-188, 362, 1993)
- Phase separation of quantum critical bubbles?



Summary & Questions

- Rise of Topology leads to a new picture of Kondo Insulators,
closer to He-3 than Silicon

- The robustness of the Surface States, Weak localization,
surface conductance and ARPES and sARPES, each suggest this is
a topological Kondo insulator.

- The high bulk resistivity makes this an excellent research
material for topological studies.

- Strong **magnetic** connection: AFM under pressure, Neutron excitons.

- Surface Kondo Breakdown: is the surface different, and can it undergo phase transitions?

- Bulk is strangely different:
breakdown, strange gapless insulator or inhomogenious quantum criticality?

- Is topology important for other strongly correlated systems - metals, superconductors?